External Technical Review for Evaluation of System Level Modeling and Simulation Tools in Support of Hanford Site Liquid Waste Process

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ABBREVIATIONS AND ACRONYMS

AES	ASPEN Engineering Suite Steady State Flowsheet Model
ACM	ASPEN Custom Modeler
ANL	Argonne National Laboratory
BARD	Bases, Assumptions, and Requirements Document
BBI	Best Basis Inventory
BBIM	BBI Maintenance Tool
BNI	Bechtel National Inc.
BOF	Balance of Facility
BVS	Bulk Vitrification System
CH-TRU	Contact-Handled Transuranic
CIO	Chief Information Officer
CIX	Cesium Ion Exchange
CRESP	Consortium for Risk Evaluation with Stakeholder Participation
CSV	Comma-separated values
DBVS	Demonstration Bulk Vitrification System
DOE	Department of Energy
DOE-SR	DOE Savannah River Operations Office
DST	Double Shell Tank
EM	DOE Office of Environmental Management
ESP	Environmental Simulation Program
ETR	External Technical Review
G2	WTP Dynamic Flowsheet (G2) Model; the Gensym software used for HTWOS and WTP Dynamic Flowsheet Models
G2MBC	G2 Mass Balance Calculator
GFSF	Glass Former Storage Facility
GPM	Glass Property Model
GUI	Graphical User Interface
HLAN	Hanford Local Area Network
HLW	High-level Waste
HLW-IPT	HLW System Integrated Project Team
HTWOS	Hanford Tank Waste Operations Simulator
HQ	Headquarters
IHLW	Immobilized HLW
ILAW	Immobilized Low-Activity Waste
IPT	Integrated Project Team
IPS	Interim Pretreatment System
KB	Knowledge Base
LAB	Analytical Laboratory
LAN	Local Area Network
LANMAS	Local Area Network Material Accounting System
LAW	Low-activity Waste
LCCM	Life-cycle Cost Model
LF	Leach Factor (caustic)

LOI	Line(s) of Inquiry
MCRs	Model Change Requests
MDD	Model Design Document
MTBF	Mean Time before Failure
MTTR	Mean Time to Repair
NMMSS	Nuclear Materials Management & Safeguards System
NNSA	National Nuclear Security Administration
OR	Operations Research
ORNL	Oak Ridge National Laboratory
ORP	Office of River Protection
PET	Process Engineering and Technology
PMB	Performance Measurement Baseline
PNNL	Pacific Northwest National Laboratory
PT[F]	Pretreatment [Facility]
QA	Quality Assurance
RAM	Reliability Availability and Maintainability
RL	Richland Operations Office
RPP	River Protection Project
SLATE	System Level Automation Tool for Enterprises (component RAM data)
SOF	Sum of Fractions
SRNL	Savannah River National Laboratory
SRS	Savannah River Site
SST	Single Shell Tank
SWPF	Salt Waste Processing Facility
TFCOUP	Tank Farm Contractor Operation and Utilization Plan
TOC	Tank Operations Contract
TPA	Tri-Party Agreement
TWINS	Tank Waste Information Network System
ULD	Unit-Liter Dose
V&V	Validation and Verification
WF	Wash Factor (water)
WFDS	Waste Feed Delivery System
WIPP	Waste Isolation Pilot Plant
WRPS	Washington River Protection Solutions
WTP	Waste Treatment and Immobilization Plant

EXECUTIVE SUMMARY

This report presents results of the External Technical Review (ETR) of the system-level modeling and simulation tools that support the planning basis for the River Protection Project (RPP), managed by the U.S. Department of Energy (DOE), Office of River Protection (ORP). A short description of each team member's and observer's relevant expertise is given in Appendix A.

The RPP mission is to retrieve and treat Hanford's tank waste and close the tank farms to protect the Columbia River. The mission involves the retrieval, treatment, and disposal of approximately 57 million gallons of radioactive waste contained in the 149 single-shelled tanks and 28 double-shelled tanks at the Hanford Site. The waste will be treated in the Waste Treatment and Immobilization Plant (WTP), which will separate the waste into high-level waste (HLW) and low-activity waste (LAW) fractions and immobilize them in glass waste forms. Modeling and simulation tools are utilized in support of the mission planning, particularly for "Optimizing the overall mission by resolution of technical and programmatic uncertainties, configuring the tank farms to provide a steady, well-balanced feed to the WTP, performing trade-offs of the required amount and type of supplemental treatment and of the amount of HLW glass versus LAW glass" [CERTA 2009a].

This review was chartered to focus on three primary areas:

- Assess the assumption that the tools used for simulation of tank waste processing yield reasonable estimates. Evaluate methods used to model facilities that are currently in either design, construction or planning stages.

- Evaluate if additional tools are needed to guide actual execution of individual processing steps.

- Evaluate the ability to timely update models as facilities in design, construction or planning stages refine their designs and operational envelopes.

The review centered on several existing software tools, including:

- **Best Basis Inventory (BBI) –** the official inventory, updated quarterly in report form, of 46 radionuclides and 26 chemicals in Hanford HLW tanks to represent current tank conditions.

- **Tank Waste Information Network System (TWINS) –** a network-accessible database that stores and provides the official characterization data for the 177 Hanford tanks including waste physical property data, sample data, and estimates of phase-based inventories and concentrations, the Best Basis Inventory; leach and wash factors for each tank; and reports that support design, operations, and planning.

- **Hanford Tank Waste Operations Simulator (HTWOS) –** a discrete-event and continuous process model developed in the Gensym G2 programming language that is used for short-term and preliminary long-term planning for the River Protection Project mission. The model simulates waste transfers and retrievals, evaporator operations, and WTP operations. HTWOS generates a dynamic mass balance of the overall lifecycle waste treatment mission.

- **WTP Dynamic Flowsheet (G2) model -** a discrete-event and continuous process model developed in the Gensym G2 programming language that is used for simulation of detailed WTP operations throughout its mission. The model utilizes the tank farm feed vector from HTWOS, applies WTP operating logic, and generates a dynamic mass balance of the plant, including cold chemical additions and volume and compositions of glass products and plant effluents.

- **Aspen Engineering Suite (AES) Steady State Flowsheet model –** a model linking Aspen Plus and Aspen Custom Modeler with OLI Alliance software that employs thermodynamic calculations to provide detailed flowsheet chemistry for time-averaged steady state cases of WTP operations.

- **WTP Operations Research (OR) model –** a discrete-event model in the WITNESS software platform that simulates material flows through the systems and subsystems of the WTP, incorporating reliability, availability and maintainability (RAM) information for operations research analysis.

Main Observations

There are four main observations:

1. ***The current System Plan relies on software tools that are limited primarily to the movement of materials. These tools currently include limited prediction of material composition, resulting in a system that is at high risk of not meeting waste acceptance criteria beyond the initial batches. There is a need for a system planning tool that provides additional details on chemistries that impact important mission parameters.***

   The G2-based models (i.e., HTWOS and the WTP Dynamic Flowsheet model) enable detailed description and projection of the physical movement of materials in tank operations and WTP processing based on current assumptions. However, these models incorporate simple expressions for chemical processes (i.e., thermodynamics, kinetics, etc.) The Aspen Steady State Flowsheet model, which does incorporate more realistic speciation and predictions, is currently limited to time averaged, steady state assumptions and applies to a small fraction of waste batches. Progress on this topic will require significant effort because it is difficult to translate elemental compositions from the Best Basis Inventory to speciated, charge-balanced feed compositions suitable for rigorous prediction in existing thermodynamic models.

2. ***Overall system analysis and optimization is limited by multiple factors, including (a) incomplete synchronization of G2-based models and (b) lack of a tool suitable for rapid analysis of different scenarios of retrieval, blending, and processing with respect to technical constraints.***

   There appears to be no technical basis to maintain two different G2-based models. Incomplete synchronization of the G2-based models for tank farm operations (HTWOS) and WTP operation (WTP Dynamic Flowsheet model) limits overall system analysis. This is because the current sets of assumptions used by the two ORP contractors are different. Critical assumptions that cause the inconsistencies between the two models include: (1) use of different feed vectors, (2) description of simplified WTP operations in HTWOS, (3) aluminum leaching/solubility, and (4) chromium removal. Because HTWOS does not implement current operational details of WTP, the system plan does not reflect the most current design or operations considerations, and, as a consequence, timely "what-if scenarios" cannot be analyzed.

   The Tank Farm Contractor Operation and Utilization Plan is based on a retrieval sequence focused on single shell tanks and farm-by-farm closure that is generated by expert staff – not by optimization using modeling and simulation tools. Because of the time required for generation of scenario input and completion of model runs, the current G2-based models – as currently configured – do not facilitate analysis of a broad range of alternative scenarios. There is a need to explore additional tools and/or approaches to enable optimization of retrieval, blending, and processing with respect to chemistry and technical constraints, such as meeting waste acceptance criteria. Such tools should also include the capability for analysis of other pretreatment options (such as at-tank or near-tank treatment) that are currently under development.

3. ***The mission has elements that are at different development stages (e.g. planning, design, construction) that require the system plan to capture uncertainties in cost, retrieval, processing, chemistry, etc. There is a need for the tools supporting the system plan to incorporate these functionalities or a new general tool is needed to capture relevant uncertainties for system planning purposes.***

   Upgraded tools and methods must include a systematic approach to uncertainty management and error propagation, and should factor in the relationship of uncertainty to cost and schedule. Modules must be developed within the current tools, or new tools must be implemented, that include cost, account for process chemistry, account for waste acceptance, and capture process changes in the pre-treatment, WTP, and future facilities.

4. ***The lack of an "overall" model that addresses the entire plant/process reliability, availability, and maintainability (RAM) for WTP and the Tank Farm hampers life-cycle analysis. There is a need to evaluate system bottlenecks and conduct "what-if" scenarios to improve process efficiency.***

   An operations research model exists for WTP developed in WITNESS software. Although there is currently not one for the tank farm, one is planned for the Waste Feed Delivery System (WFDS). Therefore, an opportunity exists for combining the operations research models (WTP and WFDS). WITNESS appears to be a flexible tool that allows adaptation in order to address process changes. Some capabilities of WITNESS software that may be useful for life-cycle analysis are not currently being used, including methods for optimization, scenarios analysis, and cost comparison of alternatives.

Recommendations

Several actions are recommended to address the observations listed above.

1. ***Recommended short-term actions (6 to 12 months) include:***
   - Improve computing resources (including processor, memory and software) as needed to reduce run times and allow more scenarios to be explored
   - Increase involvement of software engineers/modeling experts to enhance existing codes and develop more efficient computational methods
   - Develop a consistent methodology for uncertainty characterization and management among tools to facilitate analysis of error propagation, calculate overall system uncertainty and provide a sufficiently broad composition envelope for glass acceptance
   - Determine an approach for reconciling differences between assumptions in HTWOS and the WTP Dynamic Flowsheet model
   - Begin planning for the deployment of a general planning model suited for uncertainty analysis, sensitivity analysis, and feasibility/optimization of retrieval, blending, processing with respect to appropriate constraints (e.g., cost, glass properties, etc.)
   - Evaluate improved methods to approximate chemistry in the G2-based models.
     - Link to EM-20 supported activities regarding experimentation and model development for predictive chemistry, and explore options for implementation into operational and planning tools
     - Evaluate implementation of "Corporate" materials properties and BBI/TWINS databases within DOE
   - Participate in complex-wide technical exchanges to identify and adopt best practices and new software approaches
   - Work with DOE HQ and other program offices to adopt consensus standards for material properties across all models

2. ***Recommended mid-term (next 2 years) actions:***
   - Reconcile differences in assumptions between HTWOS and WTP Dynamic Flowsheet model
   - Develop a general planning model suited for uncertainty analysis, sensitivity analysis and feasibility/optimization of retrieval, blending, processing with respect to appropriate constraints (e.g., cost, glass properties, etc.)
     - Develop the capability to propagate uncertainties through the planning process
     - Begin to characterize important uncertainties
   - Develop expanded capabilities for chemical process modeling (i.e., link to EM-20 supported activities for development and implementation)
     - Thermodynamics and kinetics
     - Transient unit operations

- Implement "corporate" materials properties approach and develop "corporate" Best Basis Inventory databases
- Explore the use of software site licenses versus contractor specific ones. This could provide significant savings to DOE and improve the tools available to all contractors.
- Explore computing environments for long-term planning needs, including optimization
- Contribute to complex-wide effort to identify opportunities and approaches for system optimization

3. ***Recommended long-term (3 to 4 years) actions include:***
   - Consolidate G2-based models
   - Implement unified OR model and evaluate whether WITNESS or other tool can replace or augment some functions of the G2-based models
   - Implement general planning model including uncertainty analysis, sensitivity analysis and feasibility/optimization of retrieval, blending, processing with respect to appropriate constraints
   - Implement expanded capabilities for chemical process modeling (including improved thermodynamics and kinetics, unit operations, etc.)
   - Maintain and continue to update "corporate" materials properties and "corporate" Best Basis Inventory database
   - Continue to contribute to complex-wide effort to identify opportunities and approaches for system optimization
   - Work with DOE HQ and other program offices to adopt consensus standards for material properties across all models

External Technical Review for Evaluation of System Level Modeling and Simulation Tools in Support of Hanford Site Liquid Waste Process

1.0 Background

The Hanford Site is a 586-square-mile DOE Complex located along the Columbia River in the State of Washington used to produce nuclear material for national defense programs. Liquid wastes produced during the Manhattan Project and throughout the Cold War have been stored at the site's Tanks Farms. Approximately 57 million gallons of radioactive and chemically hazardous wastes are currently stored in 177 underground tanks located on Hanford's Central Plateau. The inventory was generated as a by-product of the recovery of plutonium from Hanford's nine nuclear reactors. Irradiated fuel from those reactors was transported to six separations facilities, where the use of multiple separation technologies resulted in a wide variety of waste compositions. In the 1950s and 1960s, approximately one million gallons of liquid radioactive waste may have been inadvertently released into the environment.

From 1944 to 1989, the liquid waste was pumped as slurry from the separations facilities through underground transfer lines and stored in underground storage tanks constructed of carbon steel. Since the separations processes operated under acidic conditions, sodium hydroxide was added to the waste streams prior to transfer to inhibit corrosion. The entrained solids settled to the bottom of the tanks, creating a bottom layer designated as sludge and leaving a clarified liquid above, the supernate. To reduce the total volume of waste stored, the supernate was periodically decanted, transferred out of waste tank farms, and evaporated. The concentrated slurry was returned to the storage tanks, where cooling resulted in formation of saltcake, a crystalline solid phase. Long-term storage at high temperatures has also resulted in the formation of a solid mass or groups of large solids that are not easily removed and so are referred to as "hard-to-remove" heels at the bottom of some tanks.

There are seven tank farms (86 total tanks) located in the 200 West area and eleven tank farms (91 total tanks) located in the East area. The tanks are of two main types: single-shell (SST) and double-shell (DST). Since 1980, the SSTs have not been in active service and most pumpable liquids have been transferred to the DSTs. As of July 2008, inventory estimates are: SSTs -- 30 Mgal and 95 MCi of radioactivity, mainly as dried sludge solids and saltcake containing entrained gases and interstitial liquids, and DSTs -- 27 Mgal and 95 MCi of radioactivity, mainly as liquids and settled solids (salts or sludge). An overall summary of the waste tanks is given in Table 1. The DST space is carefully tracked because a portion of the DST space is reserved for contingency in the event a tank leaks, and to accommodate safety operational constraints. The DSTs are an integral part of the River Protection Project (RPP) System Plan. Their mission is to:

- Support SST waste retrieval
- Support 242-A Evaporator operations
- Stage feed for delivery to the Waste Treatment Immobilization Plan (WTP)

Table 1.1 Hanford Waste Tanks Types

Type	Total Number of Tanks	Current Waste Inventory
SST	**149**	**30 Mgal**
Comments - Built from 1943 to 1964 and consists of large-capacity 133 (100 series) and 16 smaller-capacity (200 series) tanks. Assumed leaked 67. 83 are located in the West and 66 in the East 200 area. As of November 1980 all removed from active service. As of 2004 all interim (liquid removed) stabilized. As of April 2009, 7 have been retrieved, 3 have been retrieved to the limits of current technology and one is in the process.		
DST	**28**	**27 Mgal**
Comments - Built from 1968 to 1986 with an improved design and have never leaked. All tanks are currently active and subject to an integrity program. Three are located in the West and 25 in the East 200 area.		

The current plan for liquid waste processing consists of a number of highly integrated activities that require coordination among multiple contractors. Office of River Protection (ORP) manages two main contracts within the RPP system:

- The Tank Operations (TOC) Contract [DE-AC27-08RV14800] held by Washington River Protection Solutions (WRPS) includes the construction, operation, and maintenance activities necessary to store, retrieve, and transfer tank wastes; provide supplemental pretreatment for tank waste; and provide treatment, storage, and/or disposal of glass product and secondary waste streams.

- The WTP Contract [DE-AC-27-01RV14136] held by Bechtel National, Inc. (BNI) includes the design, construction, and commissioning of a pretreatment facility, two vitrification facilities (one for HLW and one for LAW), a dedicated laboratory, and supporting facilities to convert radioactive tank wastes into glass for long-term storage or final disposal.

In addition ORP interfaces with two DOE – Richland Operation Office (RL) contractors, the Mission Support Contractor and the Plateau Remediation Contractor, for waste disposal services, as well as some construction and ventilation work. Since RL is responsible for the groundwater under the tanks, it conducts the monitoring and planning. It is important to emphasize that each contractor manages facilities that are at different stages of development: (1) existing, (2) under design or construction, and (3) planned future. Alignment of program costs, scope and schedules from contractor’s plans to individual facility operations is challenging. The current system plan [CERTA 2009a] addresses these issues. Tank waste removal and treatment is a multi-year process that consists of the following steps:

1. Retrieving waste from the SSTs (*status: interim stabilized/retrieval in progress*), transferring to DSTs, (*status: operational*) and delivering the waste to WTP

2. Constructing and operating WTP. The WTP (*status: design and construction*) consists of three individual waste treatment facilities: (1) Pretreatment (PT), (2) High-Level Waste Vitrification and (3) Low-Activity Waste Vitrification.

3. Developing and deploying supplemental treatment capability is assumed to require a second LAW facility (*status: future facility*) that can safely treat about two-thirds of the LAW contained in the tank farms.

4. Developing and deploying treatment and packaging capability for Contact-Handled Transuranic (CH-TRU) tank waste (*status: early design*) for possible shipment to and disposal at the Waste Isolation Pilot Plant (WIPP) in New Mexico farms (*status: operational*).

5. Deploying interim storage capacity (*status: operational*) for the immobilized high-level waste (IHLW) pending determination of the final disposal pathway.

6. Closing the SST and DST tank farms, ancillary facilities, and all associated waste management and treatment facilities (*status: planning*).

7. Optimizing the overall mission (*status: planning*) by resolution of technical and programmatic uncertainties, configuring the tank farms to provide a steady, well-balanced feed to the WTP, performing trade-offs of the required amount and type of supplemental treatment and of the amount of HLW glass versus LAW glass.

The WTP contract covers the WTP construction and TOC contract covers the remainder, including WTP operation. The ORP mission includes the challenge of retrieving and treating Hanford’s tank waste and closing the tank farms to protect the Columbia River. Integrating facilities that are at different stages of development and managed by different contractors makes these tasks particularly challenging. The RPP seeks to accomplish this by developing an integrated system plan as shown in Figure 1.1.

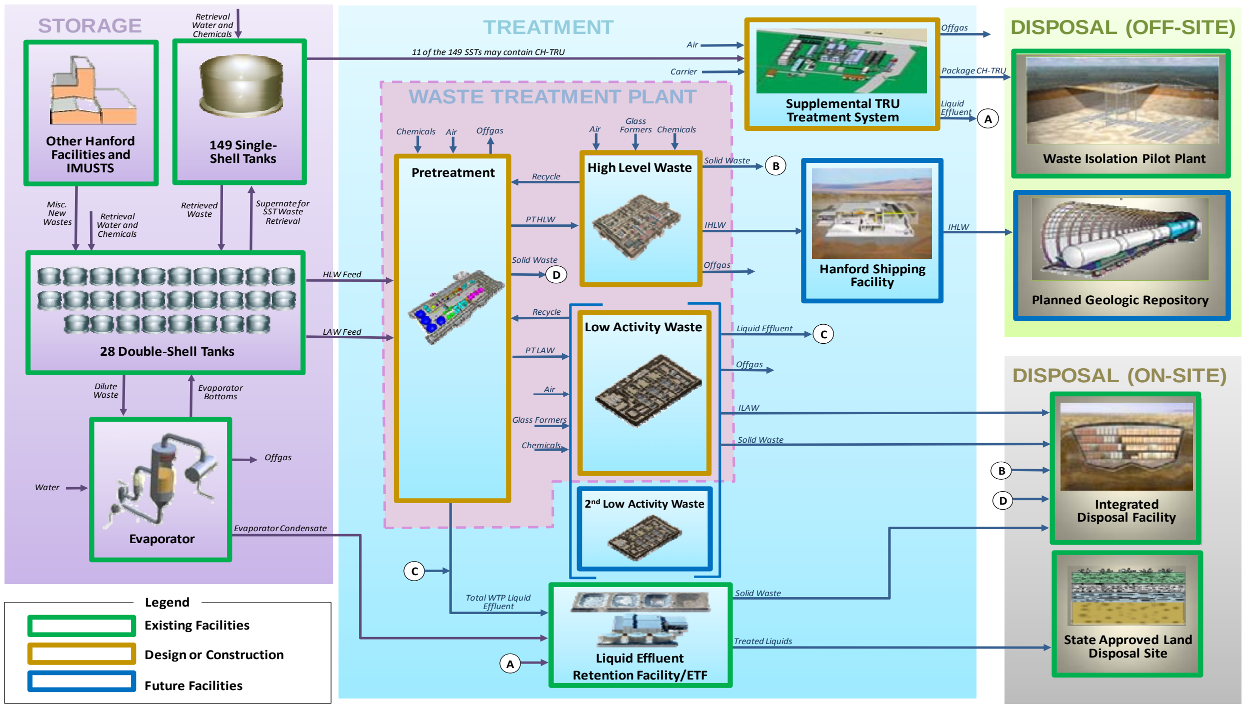


Figure 1.1 River Protection Project Simplified Flow Diagram [KIRCH 2009]

2.0 Scope of the Review

The objective of this review is to evaluate the current Process Simulation Tools that support the planning basis for the River Protection Project System Plan [CERTA 2009a]. It covers a collection of software tools used to organize and analyze information, and to guide the management and processing of high-level waste at the Hanford Site. The liquid waste system at the site is a highly integrated operation that involves a number of activities.

This review will focus on three primary areas:

- Assess the assumption that the tools used for simulation of tank waste processing yield reasonable estimates. Evaluate methods used to model facilities that are currently in either design, construction or planning stages.
- Evaluate if additional tools are needed to guide actual execution of individual processing steps.
- Evaluate ability to timely update models as facilities in design, construction or planning stages refine their designs and operational envelopes.

3.0 Team Membership

The team was comprised of five independent experts whose credentials and experience align with the specific lines of inquiry (LOI) listed in section 4.0 and who collectively provided to the team sufficiently broad capability and flexibility to address the full range of issues that emerged during the review. Technical expertise included, but was not limited to design, engineering and management of chemical processing, and computer software development. Members of the team for this review were Monica Regalbuto, Lead (EM-21), Kevin Brown (Vanderbilt University/CRESP), David DePaoli (ORNL), Candido Pereira (ANL), and John Shultz (EM-21).

Two observers from Savannah River Site participated in the review. The observers were Sonitza Blanco of (DOE-SR) and Bob Chang (SRS). Short descriptions of team members and observers relevant expertise is given in Appendix A.

4.0 Lines of Inquiry

In order to process the liquid waste at the Hanford Site, an adequate overarching strategy (master plan/schedule) that integrates all systems and operations under consideration is necessary. A systems approach ensures that all operations and interfaces, risks and alternatives are evaluated to ensure that throughput, schedule, budget, and other requirements are met. The plan must account for the variable maturity of different aspects of the project with respect to schedule and address two basic questions:

1. Is the degree of development and planning sufficient to meet the schedule for implementation?
2. What aspects of a systems approach are in place, and which aspects need further development or are missing?

The following section covers the primary LOI for the review and has been organized into three categories:

<u>Category 1: Current Overall Software Performance and Process Structure</u>

1. ***How did ORP select the various software modeling tools they are using?***
   The selection of software modeling tools used emerged logically from the intended application. The Gensym G2 programming language – used for the HTWOS and Dynamic Flowsheet models - was selected for use in simulating tank farm operations in 1991 as the result of an industry search for a platform capable of performing dynamic simulations. The majority of the elements of the TWINS database were developed by PNNL in ASP.net; the applications are being evaluated during the transfer of the TWINS database to new servers during the transition from PNNL to WRPS. The Aspen-OLI software for the Steady State Flowsheet model appears to have been selected through expert knowledge and evaluation of the capabilities of process simulators and the ability to link to thermodynamic predictive tools. The WITNESS software for OR modeling was selected to satisfy functional and performance requirements. A few of the requirements of the model include enabling the evaluation of system and overall plant reliability, quantifying relationships between glass production and equipment performance, failure, and maintenance [PEREDO]

2. ***Given the multiple contractors and stages of development of the facilities, how does ORP account for process unknowns?***
   Since many of the facilities are in design or construction stages, there are many details associated with processing the tank waste that have not been finalized. Additional, significant uncertainties exist in the tank inventories and in approximations used in predicting chemical processes (e.g., washing, leaching, etc.). The documentation of the processes to populate the data in the Best-Basis Inventory provides detailed information on how the existing

information, including sample data and process and historical knowledge were used to generate information on tank inventories and wash and leach factors. Currently, there is not a standardized and transparent approach to characterizing and documenting uncertainties in the inventory data (although uncertainties can be estimated for sample-based information in TWINS)). Bounding and intended-to-be-conservative estimates were described for Safety Analysis purposes. The expressions used for approximating chemical processes are described clearly in the documentation.

2.1. How are unknowns tracked and models updated as new information becomes available?

The model developers utilize a thorough change-control process. However, no general system or approach was described (or appears to be in-place or planned) to characterize and track uncertainties and/or unknowns that might significantly impact planning model responses. When new information becomes available that might significantly impact planning model responses and possibly decisions, there appears to be no system in place to characterize and track this information.

2.2. How are new versions of the performance measurement baseline (PMB) for the tank farm and WTP integrated?

Integration of efforts is driven by ORP. The selection of correlations, models, etc. to be used in the models is proposed by contractors and defined by ORP.

3. Has the quality of the process simulation tools been adequately assured (i.e., is the Quality Assurance (QA) plan adequate)?

The most basic element of software QA is proper process documentation. Although a comprehensive software QA review was beyond the scope of this inquiry, by reviewing the QA documentation for select models (e.g. the WITNESS OR model and HTWOS), and by reviewing the processes used by WTP/WRPS to implement their modeling programs, the team believes that in general, the simulation tools that supports the RPP have documented the proper elements of a good software QA program [PEREDO and WRPS].

One issue that was of concern, however, was the lack of citations of DOE and Industry Standards for QA in the WTP models. It appears that the WTP models are following acceptable practices regarding software documentation, but the basis on which their documentation is constructed is not explicitly tied to DOE guidance and instead seems to rely on internal contractor (e.g. Bechtel) procedures. For example, the WRPS software documentation [WRPS] explicitly mentions DOE and ASME standards. For WTP, software QA documentation and practices appear to reference additional internal contractor standards, documents, and reports. At some finer level of inspection, it might be possible to find that those contractor documents are indeed based on accepted software standards, but that is not apparent at present (i.e., a “find” query was done on related documents using the phrases “NQA” and “IEEE” yielding no results). The WTP software development process should explicitly state the standards upon which it is based, and those standards should be industry wide standards, not solely based on what the contractor believes to be a good process (though it may well be).

In addition, access to documents relevant to WTP (especially QA-related documents) was not straight forward. In general, since the document hierarchy is difficult to follow, requests for information usually resulted in the need to request another related document from WTP. As a consequence of the organization of the document control system, several iterations with site personnel where needed to obtain additional documentation. An example that illustrates this problem was seen when additional information was needed for the WITNESS model. First a formal request through ORP was required in order to receive the information the team felt was necessary for a thorough review. After the team received the requested documents approximately 2 weeks after leaving the facility, the team finds that the documents provided referenced another document that gave the rationale behind critical RAM data. The team then had to make a new specific request. A more straightforward document hierarchy and retrieval process would facilitate referencing existing information.

3.1. What is the traceability of data used to support the models?

One shortcoming common to all of the models used at the Hanford Site is the lack of a comprehensive, site-wide process to implement common data element definitions and material properties and "constants". The BBI is the starting point for tank waste characterization, but there are many more opportunities to coordinate data management and material properties (and thereby ensure appropriate traceability) across models.

3.2. Has Validation and Verification (V&V) been conducted?

Both WRPS and BNI have implemented programs to "V&V" the models they develop. One caveat is that there are technical limitations regarding the ability to V&V models for unit operations and systems that are not yet built and operational.

3.3. Are there any benchmark validation study reports?

The team did not receive any actual benchmark validation study reports from either WRPS or BNI. However, we did receive V&V reports that indicate that benchmarking (i.e. comparing against known, and accepted, model output) is being done. Also, there may be a slight variation in terminology between WRPS and BNI regarding the term "benchmark" and what that term implies. For example, WTP documentation explicitly mentions the term benchmark in their process modeling [STONE]. WRPS implies the same level and type of work, but uses the term "baseline" [KIRKBRIDE 2009b].

3.4. How are version and revision controlled?

Both WRPS and BNI have implemented version and revision control for the models they develop.

3.5. How are users instructed on software execution?

There are user manuals with instructions on how the models work, and instructions on how inputs and outputs are managed and interpreted.

4. ***How do predictions produced by previous simulation tools compare with actual process performance?***

   Only select tank farm operations are currently being conducted at the Hanford Site; the other operations (Pretreatment, WTP, etc.) needed to treat and dispose of HLW are under construction. However, laboratory and bench-scale experiments and pilot testing have been conducted to support startup of the treatment and disposal facilities. It appears that experimental data have been used to calibrate model components only, but no experimental data is being used for model validation.

5. ***How do the sites current simulation tools predictions compare with those from other tools used at other sites?***

   No formal mechanism exists to compare simulation tools predictions across DOE sites. No benchmark cases or common model predictions are compared. The authors could only compare tools, but not predictions. In general, the ORP planning tools were developed using more sophisticated software tools than those used at SRS that are used for both planning and operations. The primary platform for the ORP planning tools (i.e., HTWOS and the Dynamic WTP Flowsheet Model) is the Gensym G2 software, which is a modern, object-oriented tool. The most common tool used at SRS for planning and operations purposes is Microsoft Excel, which is primarily used by waste system experts. ORP uses the automatic transfer of information among planning models to a great degree; whereas, all data transfers for planning purposes are made manually at SRS. No efforts to benchmark software usage from other sites were identified.

   5.1. Have side-by-side comparisons been done?

   Qualitative agreement between results from HTWOS and the WTP Dynamic Flowsheet model was indicated for a limited set of runs. No examples of side-by-side comparisons with other models were presented.

6. ***Is the time required to conduct a study of model predictions acceptable for evaluation of project risks?***

   The current tools provide detailed projections of the material flows in the tank farm and WTP throughout the mission. However, it appears that there is significant opportunity for accelerating the evaluation of project risks and consideration of alternative processing approaches to reduce overall cost/risk. Although the actual setup of an HTWOS run for parametric changes takes a few days and a complete run takes about 3 – 4 hours, scope definition and assumption development for implementation of a mission scenario in HTWOS takes on the order of half a year. This limits the analysis of a broad variety of tank retrieval and processing scenarios, sequences, and assumptions. Given the magnitude of the risks in this project, it is recommended that consideration be given to the development of additional, systems-analysis tools to analyze possible improvements through variation of feed vector and implementation of additional technologies and to further evaluate risks through uncertainty/sensitivity analyses.

For the WTP OR model no explicit documentation of the time needed either to set up, run, or modify the model were observed. Anecdotal information was provided via in-room discussion during a briefing on 30 June 2009 that indicated that it could take months to significantly modify the OR model (i.e. add a unit operation) and would take days to several weeks to set up and run an existing model. The length of time being dependent on whether changes in flow parameters are needed, or the run consists of simply re-initializing the random number generator and running a model that had been run previously.

<u>Category 2: Current Individual Tools</u>

1. ***The Hanford Tank Waste Operations Simulator (HTWOS) has been identified as the center of the RPP system planning process. The model currently has some limitations. What are the effects on the System Plan Results of assumptions made in HTWOS regarding:***

    1.1. ***Waste transfer systems, not accounting for operational limitations such as transfer equipment, settling times and tank space allocations***

    The model accounts for the transfer rates associated with the particular retrieval systems in each of the tanks and assumes that transfer lines are available for all transfers at the time the transfer is initiated. The tank farms contain underground piping, valve pits, and transfer lines to facilitate the transfer between tanks and tank farms, and it is expected that transfer lines will be constructed to support retrievals before the facilities are available. There are no restrictions on the use of transfer lines based on waste types and chemistries.

    Insoluble solids retrieved from other SSTs and currently in the DST system are modeled as settling within 30 days or, in some cases, within 2 days. These assumptions are considered conservative based on data collected from specific tank wastes. Supernatant liquids decanted from LAW tanks and from dissolving LAW salts will contain suspended solids; the model assumes levels of entrained solids based on engineering judgment because direct measurement is difficult. If solids accumulate over time in a tank, it may not be possible to re-suspend them. Further, if the quantity of solids entrained in the LAW feed is excessive, separation equipment may need to be installed in the tank farms. For in-tank precipitation of Sr and TRU, gravity settling may not be adequate and additional equipment may be needed for solids-liquid separation.

    The space and function of the DSTs are assumed to be available for the duration of the cleanup mission [KIRKBRIDE 2009c]. Emergency space is reserved to store waste if there is a leak in a DST in compliance with DOE orders and to receive emergency LAW or HLW return from the WTP. Because no returns from the LAW or HLW tanks are planned, the model does not account for non-emergency returns from these tanks.

1.2. Sodium management: adding as needed for corrosion mitigation and keeping aluminum in solution, but have the effects on the overall system been evaluated?

HTWOS does not perform a caustic demand calculation to predict changes in waste chemistry or corrosion due to caustic addition though it does add the necessary NaOH and/or $NaNO_2$ to bring the waste into compliance. Supernatant liquids are diluted to 5M sodium as a conservative upper-bound to avoid solids formation. The 5M sodium limit is due to the lack of detailed SST chemistry data and likely results in the generation of higher than necessary liquid volumes during salt cake retrievals. The total sodium loading of LAW glass from pretreated feed will be determined using the 2004 DOE Model, which maximizes the sodium oxide loading in the LAW glass subject to the following constraints: 0.8 wt.% $SO3^-$ and 20 wt.% Na_2O [KIRKBRIDE 2009c]. The amount of sodium that is processed impacts the total amounts of Immobilized LAW (ILAW) that is produced, while overall sodium management impacts the time required to process the tank wastes and ultimately the time required to complete the RPP mission.

1.3. Continually changing tank farm conditions

The BBI is updated quarterly. Implementing parametric changes to HTWOS requires several days to update and run the model. Implementing changes in operating logic or new operations requires more time, weeks to months.

1.4. Determination of glass acceptability

The HTWOS model determines the glass formulation by minimizing the total mass of glass formers added to the HLW (and LAW) feed while producing a glass that meets specified property constraints. The model constrains the glass formulation to a region of known acceptable glasses and the glass properties models to applicable regions. The current HLW glass formulation model in HTWOS is the Relaxed Glass Properties Model (GPM). The LAW model is the 2004 DOE Model. [CERTA2009b] The waste loading and quantity of glass predicted by HTWOS is directly related to the glass models implemented. However, HTWOS does not account for uncertainties associated with the glass models or the waste oxide composition on which the glass is based.

1.5. Continually changing glass formulation for HLW and LAW

The large variation in waste batch compositions requires tuning of glass formulations. The HTWOS model determines the glass formulation by minimizing the total mass of glass formers added to the HLW (and specified waste loading assumptions for LAW) feed while producing a glass that meets specified property constraints. Refinements to the glass formulation envelope are focused on broadening the waste composition region and increasing waste loading although the reports and presentations did not explicitly describe how uncertainties are factored into the process.

1.6. Need for supplemental pretreatment capacity at WTP

The WTP, as configured, is not intended to process all of the tank waste. The supplemental LAW treatment facilities will process treated LAW feed from the WTP PT Facility [STONE]. Several supplemental systems under consideration have been included in the HTWOS model to assist in mission planning and scoping studies. Supplemental vitrification treatment systems in HTWOS include: Demonstration Bulk Vitrification System (DBVS), Bulk Vitrification System (BVS), East and West Supplemental LAW Treatment Plant, the Al removal Facility, and the Interim Pretreatment System (IPS).

1.7. Limitations of water chemistry models which were developed for dilute systems may not apply to current mission conditions

Dissolution of solids is predicted by water-wash factors from TWINS and by the Sr solubility model. "The use of wash factors to estimate the retrieved waste composition doesn't provide an accurate prediction of the actual waste chemistry." [KIRKBRIDE 2009c] Better predictions of chemical behavior of the wastes through detailed modeling and/or better quantification of the uncertainties associated with the predictions may have a significant impact on the RPP mission planning efforts. Detailed analysis of chemistry has been done for the WTP with the Aspen Engineering Suite (AES) for tank waste batches for which detailed thermodynamic and speciation data are available. The G2-based models utilize simple expressions for estimation of aluminum solubility in WTP that are fits to published experimental data for simple chemical systems – HTWOS uses equation 4 of CCN 160514 [REYNOLDS and ADELMUND], which is a global fit over a range of temperatures and includes an ionic strength dependence, while the WTP Dynamic Flowsheet model uses equation 9 of the same reference, which is a better fit of existing data at 25°C, but with dependence only on free hydroxide concentration. A separate External Technical Review on Hanford Tank Waste Chemistry is currently evaluating the effectiveness of those correlations; preliminary evaluation indicates that the correlation utilized in the Dynamic Flowsheet model (equation 9 of 160514) provides estimates with an acceptable level of conservatism.

1.8. Expanded operational feed envelope (outside of current range)

Implementing major changes in operating logic or new operations requires weeks to months. Once adjusted, the model typically requires 4 to 14 hours to run, depending on the scale of the case being simulated.

1.9. Simplified representation of the WTP process

The HTWOS representation of the WTP process is intended to capture all of the major operations of the WTP process flowsheet required to produce an overall system plan for the RPP mission. The simplifications in HTWOS result from the combining systems with multiple operations or identical units and reduced modeling of some process chemistries. Process upsets; downtime and maintenance are not evaluated explicitly but must be accounted for implicitly in the simplified representations. Based on comments by WRPS personnel, the waste production predicted by the HTWOS model does not differ significantly from that generated by the WTP Dynamic Flowsheet for the same feed vector. If the results are consistent for feed vectors that bracket those cases to be treated, there should be minimal effect on overall system planning. A detailed study of the impact of specific simplifications in HTWOS to differences in the results generated by the WTP Dynamic Flowsheet does not appear to have been conducted, nor has an analysis of the effect of simplifications on the propagation of uncertainties related to process chemistry and waste form production.

2. ***The HTWOS model requires input information from a variety of sources. What are the effects on the System Plan Results on assumptions made by the planning tools that provide the inputs to the model?***

   The results of the model are based on input from the BBI and TWINS, as well as near-term historical tank transfers not yet included in the current BBI. The tank inventories generated by these planning tools directly affect the results generated by HTWOS. The composition and volume of liquids and the time required to complete retrievals and transfers are necessary for the sequencing of operations between SSTs, DSTs, the tank farm evaporator and the WTP. The calculated outcomes of specified tank operations are dependent on Wash and Leach Factors assigned by TWINS and on the tank compositions generated by the BBI from TWINS. Therefore, assumptions of the behavior of solids, dissolution chemistry, chemical speciation, interstitial liquids and retrieval efficiencies, impact HTWOS results.

3. ***Does the Best-Basis Inventory (BBI), which provides waste characterization data, adequately estimate the composition and inventory of the liquid waste tanks?***

   The BBI appears to provide adequate best-estimate compositions and inventories for planning purposes when only expected operation is studied. These "best" estimates do not suffice for those evaluations needed to define the necessary compositional envelopes for operation, and thus project risk, because the waste compositions and inventories are often highly uncertain. A systematic approach to manage the uncertainties in the inventory information associated with BBI is needed.

   3.1. ***What calculations are performed?***

   The chemical composition of the waste in each of the 177 HLW tanks is calculated using three fundamental parameters (i.e., analyte concentration, waste density, and waste volume). Using these parameters, the total tank inventory as well as the phased-based concentrations and inventories are calculated. Calculations are handled differently depending upon the pedigree or type of the underlying information.

   3.2. ***What are the pertinent data needed to perform the estimation?***

   The concentrations are taken from one of three sets of information describing the waste in the tank: laboratory samples, historic Hanford tank inventory modeling (denoted "HDW Rev. 4"), or process knowledge. The density used is either the sample density from the laboratory, the HDW Rev. 4 density, or an average density of the various component layers in the waste. The final parameter represents the current estimate of the volume of the component layer. Combinations of the concentrations (and corresponding densities) are allowed. In general, uncertainties in these parameters are not estimated or propagated through the models using the BBI.

3.3. How is gas generation calculated

The hydrogen gas generation is computed in the Dynamic WTP Flowsheet model for 13 selected vessels and the evaporator based on a set of 13 compounds that contribute to hydrogen generation depending upon conditions [DENG 2009]. The six major alpha emitting radionuclides and eight primary beta/gamma emitters are accounted for as providing the radiolysis driver for hydrogen generation. The impact of nitrate and nitrite on reducing the generation is also accounted for in the prediction. The contribution from thermolysis is included based on the estimated aluminate concentration. The total hydrogen produced is then the sum of the radiolysis and thermolysis impacts. The model appears to adequately predict the hydrogen generation rate for planning purposes although only the worst case conditions are used (i.e., not uncertainties) for these calculations to reduce the computational burden [DENG 2009]. The hydrogen generation calculations in HTWOS were found to agree with those in the WTP Dynamic Flowsheet model [KIRKBRIDE 2009b].

4. Do the water-wash and caustic-leach factors adequately estimate the composition and inventory of the washes resulting from each sludge batch?

It was generally agreed upon that there are very large uncertainties associated with the water-wash and caustic-leach factors. These factors are currently based on experimental data for limited conditions that may or may not adequately represent those in the Hanford tanks and/or in the future leaching processes in the WTP. Because the uncertainties in these factors are not propagated through the models or planning process, there is no way of telling whether or not these factors are indeed adequate to provide compositions relevant for planning purposes. A program is underway to perform additional experiments and to revise or replace these factors with more accurate representations based on available thermodynamic codes and databases.

4.1. What calculations are performed using these factors?

The water-wash and caustic-leach factors are zero-order approximations of the complex solid-liquid equilibrium that occurs in the waste during processing [CERTA 2008]. These factors essentially provide “splits” between the solid and liquid phases in the wastes for analytes (and their isotopes) selected for their potential impact on HLW glass produced. These factors are used in the ORP planning tools including HTWOS and the WTP Dynamic Flowsheet model.

4.2. What are the pertinent data needed to perform the estimation?

The water-wash and caustic-leach factors are used to distribute the inventory of selected analytes (and corresponding isotopes) between the liquid and solids phases based on their respective masses. These factors are zero-order approximations that apply only to the specific set of conditions used when they were developed. For example, the water-wash factors describe the solubility of the tank waste when contacted with large quantities of water and cannot accurately reflect “complex changes in solid-liquid equilibrium that occur as varying amounts of water are used during retrieval, that occur when mixing different wastes, or that occur from concentration (removal of water) in the 242-A Evaporator or in the WTP." [CERTA 2008] Additional experiments and bench-scale and pilot testing supported by chemistry modeling are needed to provide a more defensible method for estimating solubilites for both water washing and caustic leaching processes.

5. ***How does the Tank Waste Information Network System (TWINS) evaluate the BBI, water wash and caustic leach factors and the supplemental characterization data for use by HTWOS?***

   TWINS has a built-in function called Resolve that allows the user to review, qualify, and flag data that are used in estimating inventories. The Best-Basis Inventory function allows the user to examine the tank characterization data's pedigree and to select the most appropriate and accurate information for the BBI calculations before use in modeling. However, these functions are not automated when generating the inventory and wash and leach factors used in HTWOS. Familiarity with the system appears to be needed to evaluate the data used.

6. ***What is the confidence level of the feed vectors generated by HTWOS for input to WTP Dynamic Model (G2) and how is this confidence tracked?***

   There does not appear to be any assignment of confidence levels to the feed vectors generated by HTWOS. Neither of the G2-based models assigns uncertainties to chemical values or Wash and Leach Factors nor do they track the propagation of uncertainty through the model, as currently configured. The G2 Mass Balance Calculator (G2MBC) [DENG] adjusts the feed vector composition obtained from HTWOS, performing a charge balance on the input composition and adding any new components required for WTP operations.

7. ***The WTP G2 model is used for analysis and assessment of WTP operations: equipment utilization, reagent demand, process and facility design options, integration with tank farms and waste acceptance. If designs are frozen for regulatory license acquisition, how are these results used?***

   The uncertainties associated with the processing of the tank wastes will necessitate that WTP operations remain flexible even after designs are finalized. Processing will undoubtedly change as the WTP begins operations and starts treating liquids (and solids) derived from actual tank wastes. Waste acceptance criteria analysis can possibly be incorporated into the WTP Dynamic Flowsheet model in order to more closely tie the acceptability constraints on the IHLW to the processing that ultimately generates the vitrified forms. If modeling of the detailed chemistry using AES becomes feasible for a wider array of tank waste batches, the ultimate use of the WTP Dynamic Flowsheet model would be re-evaluated.

8. ***What is the relationship between HTWOS and G2?***

   HTWOS is a dynamic model used to test specific tank waste retrieval flowsheets and to assist in planning of transfers, evaporator operations, and the WTP; it is used for overall project planning. As one of its functions, the HTWOS code generates the feed vector for the WTP Dynamic Flowsheet model. The WTP Dynamic Flowsheet model ("G2-based") is a dynamic model used to simulate detailed operations over the entire WTP. Both codes model the WTP, but the WTP model within HTWOS, though operationally consistent with that in the

Dynamic Flowsheet model, is simplified as the scope of the model is broader. Since WTP operations are the focus of the Dynamic Flowsheet model, the WTP flowsheet is modeled in greater detail. Both models are written in the Gensym G2 software. HTWOS was the initial starting point in the development of the WTP Dynamic Flowsheet model, but the methodologies used for the two models have diverged significantly. Ideally HTWOS should be aligned with the WTP process flowsheet. Currently this is not the case, as HTWOS is always one design step behind.

9. ***Is the output of models provided in a user friendly format (Graphical User Interface)?***
   HTWOS saves model files, supporting data, and results at the end of each run. The run data is saved in 37 knowledge base (KB) files, and the model version is saved as a snapshot file. The HTWOS model generates 12 formatted Excel spreadsheets tailored to specific end-users. The code also generates charts and comma-separated values (CSV) text files as output. The WTP Dynamic Flowsheet model places output data in an Oracle database with limited user manipulation required. The output is processed using Oracle and Matlab, and is in a form conducive to export to Excel spreadsheets. The AES model generates data in Excel worksheet files, providing stream and process composition data. Successful model runs are saved as Aspen Backup files. Several functions within the Aspen Suite also allow the user to save process snapshots for analysis or flowsheet development. Both G2-based models and AES use object-oriented programming, enabling the user to access stream and unit operation information directly via the flowsheet graphics.

Category 3: Additional Tools Needed

1. ***Are all critical processing steps characterized?***
   Although all critical processing steps are characterized in the HTWOS and WTP models, the characterization is not the best representation of the system. Simple models of chemistry in these tools do not enable full accounting for thermodynamic and kinetic variations. Updates to the code to reflect design changes are an elaborated process, especially when new unit operations are needed.

2. ***Is the current equipment available, number of licenses purchased, number of trained personnel adequate to perform the scope of modeling needed?***
   A general planning model is needed that is suited for uncertainty analysis, sensitivity analysis and feasibility/optimization of retrieval, blending, processing with respect to appropriate constraints (e.g., cost, glass properties, etc.). The Hanford waste management system could benefit from coordinating modeling efforts between WRPS (tanks) and BNI (WTP). There is no technical reason for two G2 based models or two OR models (one for the tank side and one for the treatment side). Contractual arrangements (e.g. personnel, data access, equipment access, model access, etc.) necessary to coordinate this effort should be pursued by ORP management. In addition, a coordinated approach to data element definitions and data properties definitions (via a common database system) would benefit all models on the site. The final step in improving lifecycle modeling would be to implement an overall systems modeling tool (or modification or addition to existing tools) to incorporate costs, budget, and schedule impacts for the entire lifecycle. The use of software Site licenses versus contractor

specific ones will provide significant savings to DOE and improve the tools available to all contractors.

5.0 Overall System Observations and Recommendations

The RPP System Plan establishes the planning basis for activities to be conducted to retrieve and treat Hanford's tank waste and close the tank farms. Process activities include: (1) storage of radioactive waste in underground tanks, (2) removal and treatment of waste, (3) vitrification of low-activity and high-level for disposal, and (4) storage of the vitrified waste prior to permanent disposition.

The scope of the review was to evaluate the current process simulation tools that support the planning basis for the RPP System Plan to assess if the modeling and simulation tools used yield reasonable estimates of the operations and timetables required to complete all liquid waste treatment activities. Based on a review of the relevant software tools on hand, the team evaluated the adequacy of the available tools and the need for development of additional tools. Finally, the team evaluated methods that can improve the rate at which system model predictions are performed. The findings of this review overlap the three primary lines of inquiry. Therefore, the findings may not directly correspond one to one with the scope questions listed in the Charter given in Appendix B.

5.1 Main Observations

There are four main observations:

1. ***The current System Plan relies on software tools that are limited primarily to the movement of materials. These tools currently include limited prediction of material composition, resulting in a system that is at high risk of not meeting waste acceptance criteria beyond the initial batches. There is a need for a system planning tool that provides additional details on chemistries that impact important mission parameters.***

   The G2-based models (i.e., HTWOS and the WTP Dynamic Flowsheet model) enable detailed description and projection of the physical movement of materials in tank operations and WTP processing based on current assumptions. However, these models incorporate simple expressions for chemical processes (i.e., thermodynamics, kinetics, etc.) The Aspen Steady State Flowsheet model, which does incorporate more realistic speciation and predictions, is currently limited to time averaged, steady state assumptions and applies to a small fraction of waste batches. Progress on this topic will require significant effort because it is difficult to translate elemental compositions from the Best Basis Inventory to speciated, charge-balanced feed compositions suitable for rigorous prediction in existing thermodynamic models.

2. ***Overall system analysis and optimization is limited by multiple factors, including (a) incomplete synchronization of G2-based models and (b) lack of a tool suitable for rapid analysis of different scenarios of retrieval, blending, and processing with respect to technical constraints.***

   There appears to be no technical basis to maintain two different G2-based models. Incomplete synchronization of the G2-based models for tank farm operations (HTWOS) and WTP operation (WTP Dynamic Flowsheet model) limits overall system analysis. This is because the current sets of assumptions used by the two ORP contractors are different. Critical assumptions that cause the inconsistencies between the two models include: (1) use of different feed vectors, (2) description of simplified WTP operations in HTWOS, (3) aluminum leaching/solubility, and (4) chromium removal. Because HTWOS does not implement current operational details of WTP, the system plan does not reflect the most current design or operations considerations, and, as a consequence, timely "what-if scenarios" cannot be analyzed.

The System Plan is based on a retrieval sequence strategy focused on single shell tanks and farm-by-farm closure that is generated by expert staff – not by optimization using modeling and simulation tools. Because of the time required for generation of scenario input and completion of model runs, the current G2-based models – as currently configured – do not facilitate analysis of a broad range of alternative scenarios. There is a need to explore additional tools and/or approaches to enable optimization of retrieval, blending, and processing with respect to chemistry and technical constraints, such as meeting waste acceptance criteria. Such tools should also include the capability for analysis of other pretreatment options (such as at-tank or near-tank treatment) that are currently under development.

3. ***The mission has elements that are at different development stages (e.g. planning, design, construction) that require the system plan to capture uncertainties in cost, retrieval, processing, chemistry, etc. There is a need for the tools supporting the system plan to incorporate these functionalities or a new general tool is needed to capture relevant uncertainties for system planning purposes.***

   Upgraded tools and methods must include a systematic approach to uncertainty management and error propagation, and should factor in the relationship or uncertainty to cost and schedule. Modules must be developed within the current tools, or new tools must be implemented, that include cost, account for process chemistry, account for waste acceptance, and capture process changes in the pre-treatment, WTP, and future facilities.

4. ***The lack of an "overall" model that addresses the entire plant/process reliability, availability, and maintainability (RAM) for WTP and the Tank Farm hampers life-cycle analysis. There is a need to evaluate system bottlenecks and conduct "what-if" scenarios to improve process efficiency.***

   An operations research model exists for WTP developed in WITNESS software. Although there is currently not one for the tank farm, one is planned for the Waste Feed Delivery System (WFDS). Therefore an opportunity exists for combining the operations research models (WTP and WFDS). WITNESS appears to be a flexible tool that allows adaptation in order to address process changes. Some capabilities of WITNESS software that may be useful for life-cycle analysis are not currently being used, including methods for optimization, scenarios analysis, and cost comparison of alternatives.

5.2 System Planning Modeling Tools

The output from a collection of multi-use software tools is required to support system planning. These tools are also used to provide operational support. The modeling tools currently used by the Hanford Site liquid (and solids) waste system planning are summarized in Figure 5.2.1 and Table 5.2.1. These tools include:

- **Best Basis Inventory (BBI) –** the official inventory, updated quarterly in report form, of 46 radionuclides and 26 chemicals in Hanford HLW tanks to represent current tank conditions.

- **Tank Waste Information Network System (TWINS) –** a network-accessible database that stores and provides the official characterization data for the 177 Hanford tanks including waste physical property data, sample data, and estimates of phase-based inventories and concentrations, the Best Basis Inventory; leach and wash factors for each tank; and reports that support design, operations, and planning.

- **Hanford Tank Waste Operations Simulator (HTWOS) –** a discrete-event and continuous process model developed in the Gensym G2 programming language that is used for short-term and preliminary long-term planning for the River Protection Project mission. The model simulates waste transfers and retrievals, evaporator operations, and WTP operations. HTWOS generates a dynamic mass balance of the overall lifecycle waste treatment mission.

- **WTP Dynamic Flowsheet (G2) model -** a discrete-event and continuous process model developed in the Gensym G2 programming language that is used for simulation of detailed WTP operations throughout its mission. The model utilizes the tank farm feed vector from HTWOS, applies WTP operating logic, and generates a dynamic mass balance of the plant, including cold chemical additions and volume and compositions of glass products and plant effluents.

- **Aspen Engineering Suite (AES) Steady State Flowsheet model –** a model linking Aspen Plus and Aspen Custom Modeler with OLI Alliance software that employs thermodynamic calculations to provide detailed flowsheet chemistry for time-averaged steady state cases of WTP operations.

- **WTP Operations Research (OR) model –** a discrete-event model in the WITNESS software platform that simulates material flows through the systems and subsystems of the WTP, incorporating reliability, availability and maintainability (RAM) information for operations research analysis.

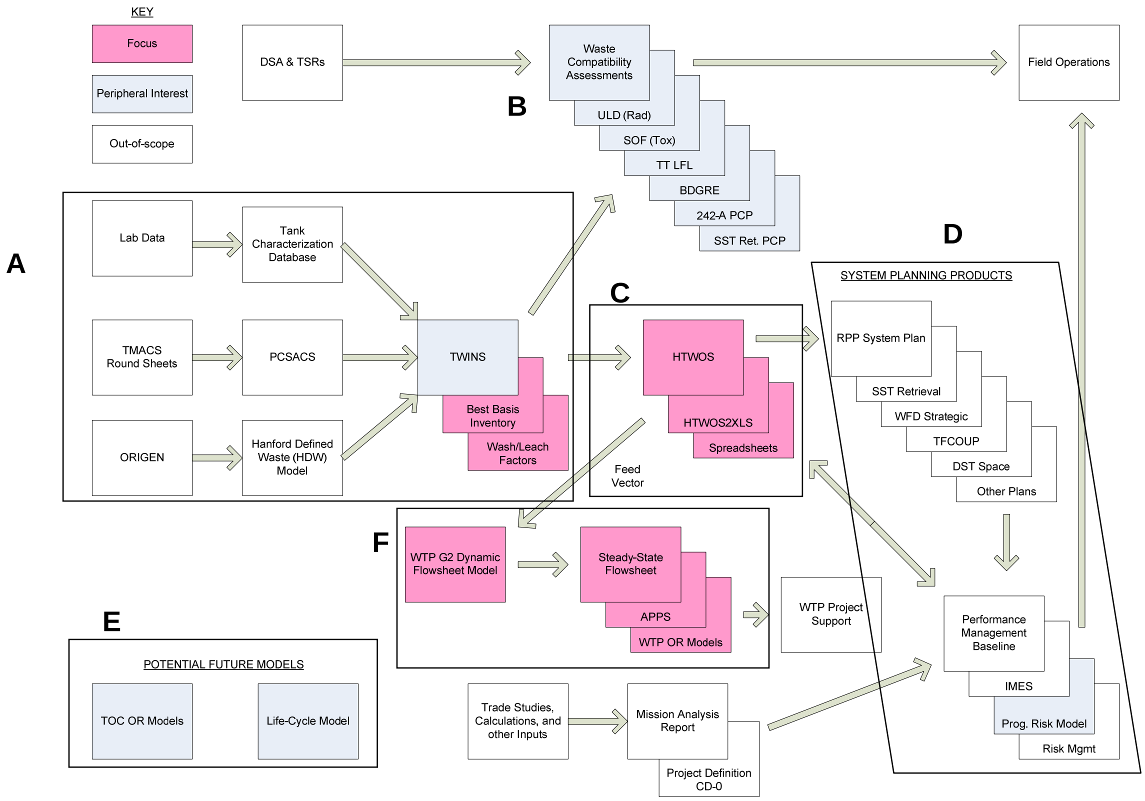


Figure 5.2.1 Overview of ORP Liquid Waste System Planning Modeling Tools

The software tools provide data that are used as the basis for several key functions including safety basis, tank operations, system planning, WTP planning, and waste acceptance. The roles of these software tools and information flows between tools are outlined below.

<u>Tank Inventory Information</u>
- Best Basis Inventory (BBI)
- Tank Waste Information Network System (TWINS)

<u>Implement Safety Basis for Operations</u>
- Waste Compatibility Assessment (WCA)
- Unit Liter Dose (ULD) radiological source term
- Unit Sum of Fractions (SOF) toxicological source term
- Time to Lower Flammability Limit (TTLFL)
- Buoyant Displacement Gas Release Event (BDGRE)

<u>Tools for Tank Operations System Planning</u>
- Hanford Tank Waste Operations Simulator (HTWOS)

<u>System Planning Products</u>
- ORP Project System Plan
- Retrieval Plan
- Tank Farm Contractor Operation and Utilization Plan (TFCOUP)

WTP Planning Tools

- Dynamic (G2) Flowsheet
- ASPEN Steady State Model (AES)
- Operational Research (OR) models

Potential Future Tools

- Operational Research (OR) models for Tank Farms
- Overall Life-Cycle Model

Input/output information to/from these tools is in multiple formats, with a minimum of manual input. Approaches for tank inventory material transfers, transmission of information to safety basis activities, and to planning tools are effective. Model and software configuration management is effective. Information transfer between codes and automated report preparation is efficient. Data is properly archived.

Table 5.2.1 Summary of Current Hanford Liquid Waste System Planning Modeling Tools

	Best Basis Inventory (BBI)	Tank Waste Information Network System (TWINS)	Hanford Tank Waste Operations Simulator (HTWOS)	WTP Dynamic Model (G2)	AES Steady State Flowsheet Model	WTP Operations Research (OR) Model
Description	MS Word Document and Excel (best estimate tank inventories)	Database and Dozens of ASP.net Applications (tank characterization data)	Gensym G2 Object-Oriented System (simulate RPP mission)	Gensym G2 Object-Oriented System (discrete-time material balance calculations)	Aspen Engineering Suite (process flowsheet material balance)	WITNESS Discrete-event simulation model (Operations Research analysis of WTP)
Function	Planning Supports Design Operation Support	Planning Supports Design Operation Support	Planning Operations Support (Short-term)	Planning	Flowsheet Validation Supports Safety Analysis	Planning
Inputs	Samples, process knowledge, historical transfer data, waste templates	BBI, SACS database, OMNI-LIMS	BBI (inventory) via TWINS, TWINS (wash and leach factors), scenario, HTWOS MDD, WTP BARD and WTP MDD	Feed vector, scenario, WTP BARD and MDD	Reconciled (i.e., speciated/charge-balanced) tank chemistries, OLI (ESP), WTPBASE	Process times, tank capacities, flowrates, operating rules, RAM data, step times
Outputs	Tank characterization data, criticality data tracking	Tank characterization and best basis inventory reports and spreadsheets	Feed vector, custom spreadsheets as input to System Plan	Volume, solids, composition , predicted glass properties by process stream	Compositions (speciated) and physical properties by stream	Reliability results (e.g., availability, usage v. idling, broken/repair times)
QA*	Level F	Level B (ULD/SOF currently Level A)	Level F	Level F	Level F	Level F

* Software grading levels are based primarily on the impact a failure of the software has on the failure of an operating system. The software grade levels that require the most stringent QA requirements are levels "A" (highest), "B", and "C". Software graded at those levels implies that the failure of the software has the possibility to impact nuclear safety systems and/or impact regulatory compliance requirements. The lowest grade of software is level "F". (DOE G 414.1-4, 6-17-05, "SAFETY SOFTWARE GUIDE for USE with 10 CFR 830 Subpart A, Quality Assurance Requirements, and DOE O 414.1C, Quality Assurance")

5.3 Overall Recommendations

The ORP contractors currently use modern, object-oriented tools to provide detailed projections of the material flows in the tank farm and WTP throughout the mission. However, there is opportunity for significant savings and process improvement through integration of systems and enhanced systems modeling. Figure 5.3.1 depicts recommended elements of an upgraded set of system tools for support of planning and operations. The primary differences from the current approach (see Figure 5.2.1) are: reductions in the number of models (i.e., combine and unify the G2-based models, and establish a single, unified operations research model); addition of a high-level system planning model; and incorporation of uncertainty information for planning.

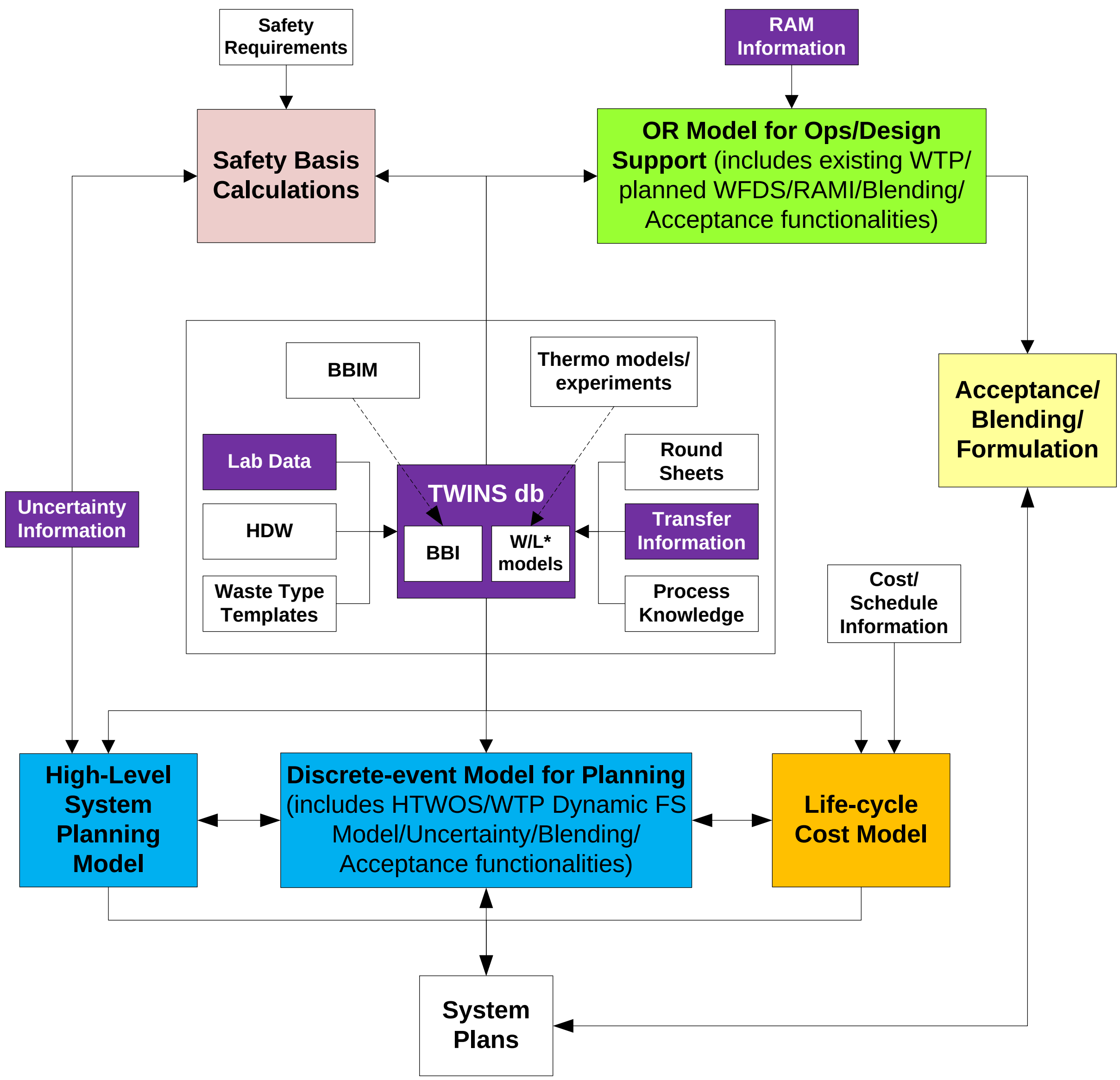


Figure 5.3.1 Recommended Integrated Planning and Development Tools

The largest opportunity for improvement is in development of a high-level planning model. Such a model would accelerate the evaluation of project risks and consideration of alternative processing approaches to reduce overall cost/risk. The mission scenario in the current System Plan is based on a retrieval sequence using a strategy that is generated by expert staff using limited iterations of HTWOS runs – not by rigorous optimization. Currently, capability for analysis of tank retrieval and processing scenarios, sequences, and assumptions is limited; for instance, scope definition and assumption development for implementation of a mission scenario in HTWOS takes on the order of half a year due to organizational approval requirements. Given the magnitude of the costs and risks of the ORP mission, it is strongly recommended that consideration be given to the development of additional, systems-analysis tools to allow uncertainty analysis, sensitivity analysis and feasibility/optimization of retrieval, blending, and processing (both baseline and alternative) with respect to appropriate constraints (e.g., cost, glass properties, etc.) for the development and evaluation of alternative mission scenarios. Benefits would include:

1. Saving overall processing time through optimization
2. Understanding the life-cycle risks and benefits of alternative processing scenarios
3. Developing optimization strategies and consideration of alternative optimization objectives (e.g., minimize HLW canister production vs. minimize processing time, etc.)
4. Avoiding unnecessary orphan waste streams prior to the end of processing

The high-level planning modeling capability could potentially be developed through multiple routes, such as:

- An integrated expansion of an enhanced HTWOS model, ported as needed to suitable computational hardware (clusters or large-scale computing) for accelerated operation and optimization
- An expansion of the operational research model under development
- A new tool, utilizing existing process simulation, optimization and uncertainty assessment methodologies

ORP is encouraged to pursue development of a planning model and work with EM-20 to evaluate alternative options. Enhancement of ORP system planning tools should be done in concert with Complex-wide integrated planning development. Development of ORP system tools should be aligned with the overall High-Level Waste System Integrate Project Team (HLW-IPT) goals for development of a life-cycle cost model (LCCM). The LCCM will take data from SRS and ORP tank inventories and discrete-event modeling tools to evaluate scenarios to reduce cost and identify technical needs.

Specific recommendations based on the listed observations for implementation within the next 6 to 12 months (short-term), 2 years (mid-term) and 3 to 4 years (long-term) are given below:

1. ***Recommended short-term actions (6 to 12 months) include:***
   - Improve computing resources (including processor, memory and software) as needed to reduce run times and allow more scenarios to be explored

- Increase involvement of software engineers/modeling experts to enhance existing codes and develop more efficient computational methods
- Develop a consistent methodology for uncertainty characterization and management among tools to facilitate analysis of error propagation, calculate overall system uncertainty and provide a sufficiently broad composition envelope for glass acceptance
- Determine an approach for reconciling differences between assumptions in HTWOS and the WTP Dynamic Flowsheet model
- Begin planning for the development of a general planning model suited for uncertainty analysis, sensitivity analysis, and feasibility/optimization of retrieval, blending, processing with respect to appropriate constraints (e.g., cost, glass properties, etc.)
- Evaluate improved methods to approximate chemistry in the G2-based models.
    - Link to EM-20 supported activities regarding experimentation and model development for predictive chemistry, and explore options for implementation into operational and planning tools
    - Evaluate implementation of “Corporate” materials properties and BBI/TWINS databases within DOE
- Participate in complex-wide technical exchanges to identify and adopt best practices and new software approaches
- Work with DOE HQ and other program offices to adopt consensus standards for material properties across all models

2. ***Recommended mid-term (next 2 years) actions:***
    - Reconcile differences in assumptions between HTWOS and WTP Dynamic Flowsheet model
    - Develop a general planning model suited for uncertainty analysis, sensitivity analysis and feasibility/optimization of retrieval, blending, processing with respect to appropriate constraints (e.g., cost, glass properties, etc.)
        - Develop the capability to propagate uncertainties through the planning process
        - Begin to characterize important uncertainties
    - Develop expanded capabilities for chemical process modeling (i.e., link to EM-20 supported activities for development and implementation)
        - Thermodynamics and kinetics
        - Transient unit operations
    - Implement “corporate” materials properties approach and develop “corporate” Best Basis Inventory databases
    - Explore the use of software site licenses versus contractor specific ones. This could provide significant savings to DOE and improve the tools available to all contractors.
    - Explore computing environments for long-term planning needs, including optimization
    - Contribute to complex-wide effort to identify opportunities and approaches for system optimization

3. ***Recommended long-term (3 to 4 years) actions include:***
    - Consolidate G2-based models
    - Implement unified OR model and evaluate whether WITNESS or other tool can replace or augment some functions of the G2-based models

- Implement general planning model including uncertainty analysis, sensitivity analysis and feasibility/optimization of retrieval, blending, processing with respect to appropriate constraints
- Implement expanded capabilities for chemical process modeling (including improved thermodynamics and kinetics, unit operations, etc.)
- Maintain and continue to update “corporate” materials properties and “corporate” Best Basis Inventory database
- Continue to contribute to complex-wide effort to identify opportunities and approaches for system optimization
- Work with DOE HQ and other program offices to adopt consensus standards for material properties across all models

6.0 Individual Tools Observations and Recommendations

This section covers each of the current tools used for the RPP System Plan. For each of the tools a brief description is given, followed by observations and short-term, mid-term and long-term recommendations. The time table for each of these recommendations is the same as for the overall recommendations given in Section 5.0. Short-term is within the next 6 to 12 months, mid-term within the next 2 years and long-term within the next 3 to 4 years.

6.1 Best Basis Inventory

Description

The Best Basis Inventory (BBI) is the official source (in report form) for tank waste inventory estimates at the Hanford Site [PLACE, CERTA 2008]. This report provides tank waste composition data for 26 chemical and 46 radionuclides in the 177 underground waste storage tanks for safety analyses; risk assessments; and waste retrieval, treatment, and disposal operations as illustrated in Figure 6.1.1. Over 100 additional analytes, generally obtained on an opportunistic basis, are tracked and reported via the Tank Waste Information Network System when available [SASAKI 2001a]. TWINS is described in the following section. The estimates contained in the BBI are based on best “available” information to describe tank waste contents and are not intended to be bounding, to include uncertainty, or to reconcile chemical behavior. The information used includes core, auger, and grab sample information, when available, process knowledge and waste type templates. The development and maintenance of the BBI is an ongoing effort [SASAKI 2001a]. Inventories for waste tanks are updated quarterly using new sample data, waste transfers, and additional process knowledge.

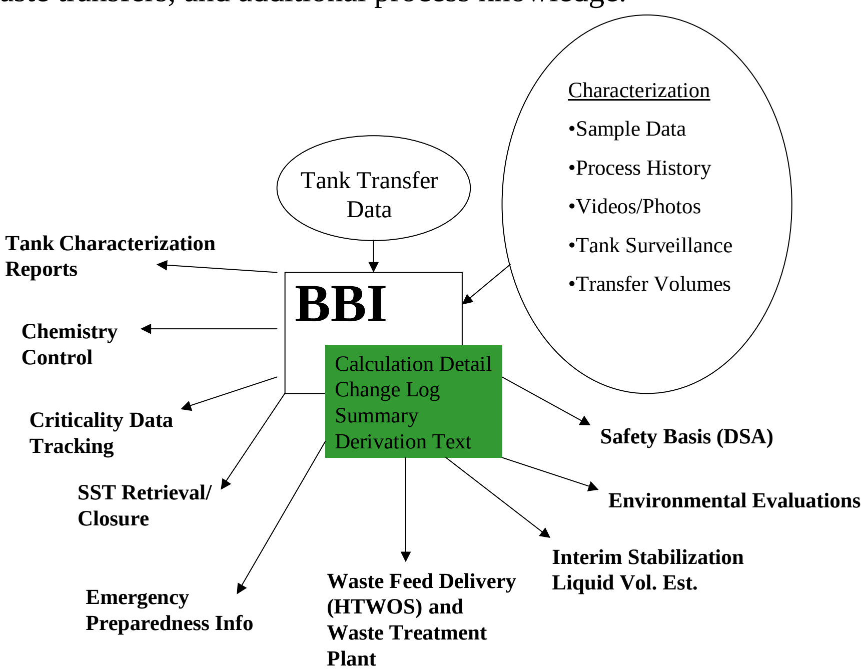


Figure 6.1.1 BBI Inputs and Applications [PLACE]

The BBI Program was chartered to develop a standardized inventory of chemicals and radionuclides stored in the 177 underground tanks. As illustrated in Figure 6.1.2, “best-estimate” inventories are developed from tank sample data or, in lieu of sample data, from engineering calculations. One of the primary engineering calculations is to estimate the volumes of waste layers in a tank and combine these with the estimated compositions of the tank waste layers (i.e., denoted “waste type templates”) [SASAKI 2001b].

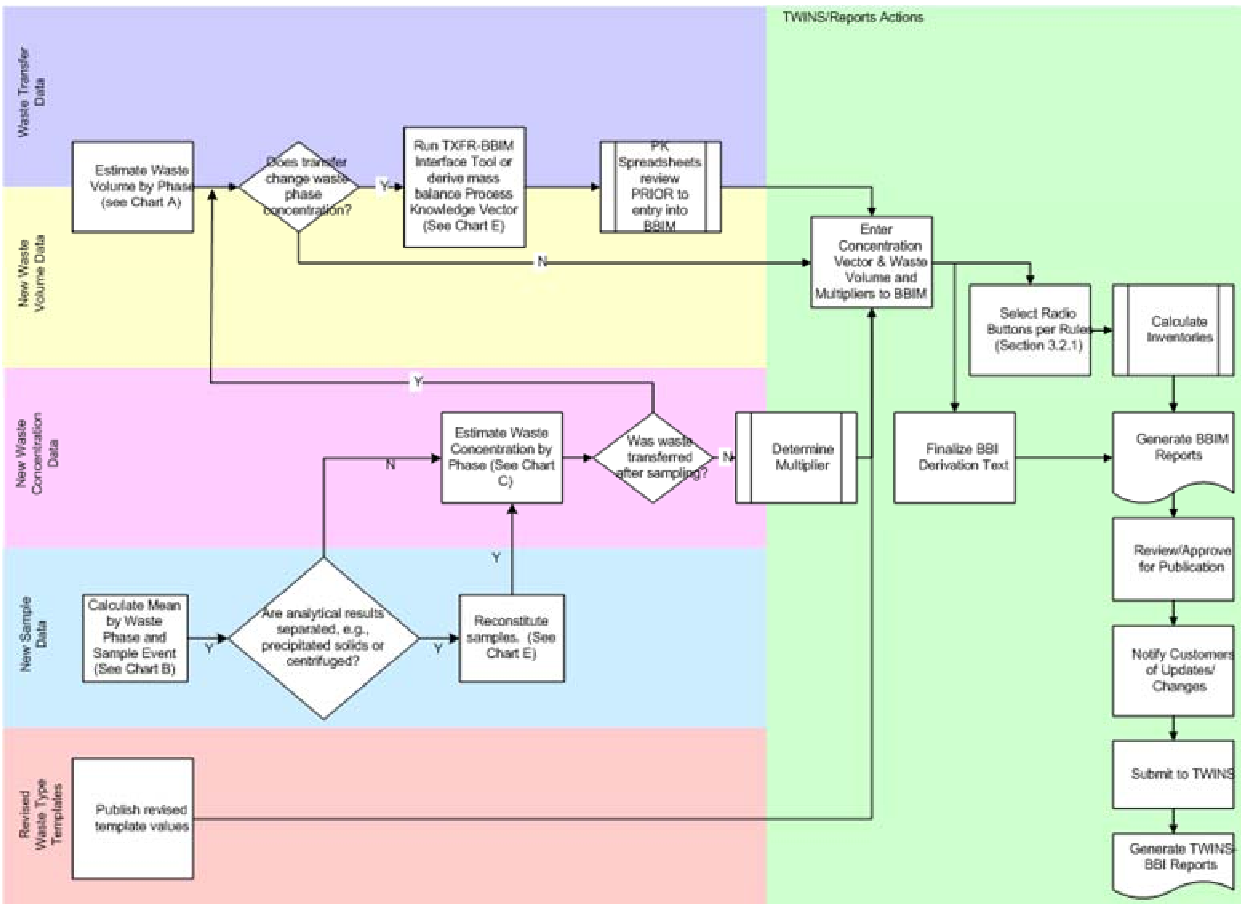


Figure 6.1.2 BBI Process Flow Chart [PLACE]

Many of the calculations used to develop the BBI are performed using the Best Basis Inventory Maintenance Tool (BBIM), which uses a set of four databases with built-in calculations to model the chemical composition of the Hanford tank wastes [TRAN]. Three fundamental parameters (i.e., analyte concentration, waste density, and waste volume) are used to calculate total waste inventories, phased-based inventories, and phased-based concentrations for selected constituents in each of the 177 tanks as illustrated in Figure 6.1.3. The BBIM structure was designed to represent the expected structure of the wastes in the tank to provide the ability to describe tank waste and to develop meaningful queries and reports in support of tank waste analysis and tank farm operations [TRAN]. The Best-Basis Inventory Maintenance Tool (BBIM) was not described to the review team before or during the ORP site visit nor was any documentation provided.

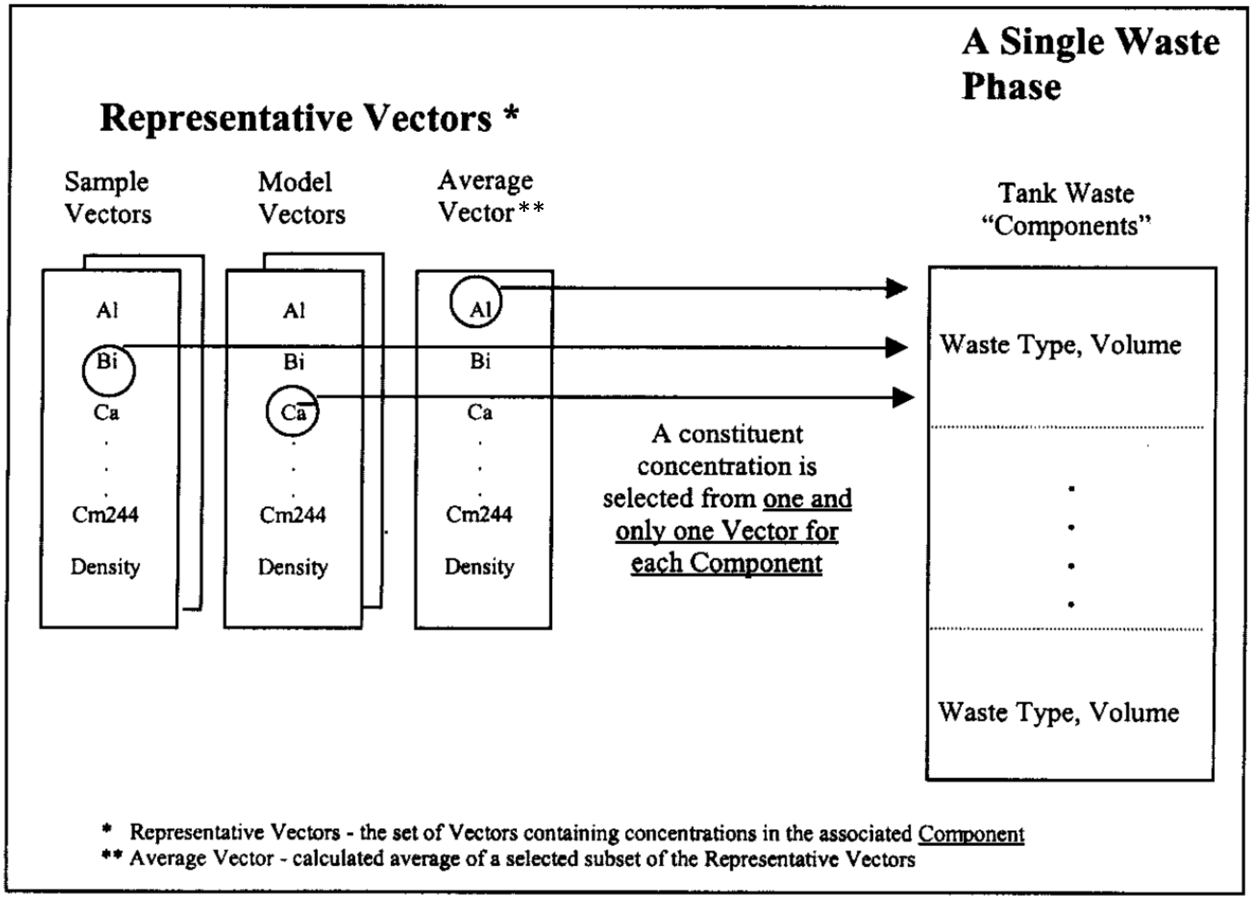


Figure 6.1.3 Physical Waste Representation in the BBIM [TRAN]

Observations

The information available to the review team indicates that the calculations underlying the generation of best-estimate tank inventories using sample information, process knowledge, and waste type templates is reasonable. Sample-based templates are not available for all waste types nor have all tanks been sampled; however, the waste types not represented by templates are likely minor contributors and qualitative agreement has been reached on waste types for the 132 waste tanks that have been sampled of the total 177 tanks. Although qualitative agreement has been reached for the majority of tanks based on sample information, quantitative estimates for the concentrations developed using the templates may be off by possibly an order of magnitude due to sampling and heterogeneity issues.

The BBI uses fundamental parameters (i.e., analyte concentration, waste density, and waste volume) to calculate total waste inventories as well as inventories and concentrations by layer (i.e., sludge, salt cake, and supernate) for selected constituents in each of the 177 tanks. Each tank often must be considered individually (i.e., there are few "cross-cutting" assumptions) when estimating inventories by layer. These inventories are provided based on simple chemical formulae (i.e., are not speciated), which makes it difficult to translate BBI concentrations to speciated, charge-balanced feed compositions suitable for rigorous thermodynamic prediction.

The inventory estimates in the BBI are intended to be “best estimate” in nature. These estimates are directly used in planning or adjusted before use in Safety Analysis (i.e., conservatism is added to provide bounding estimates). Uncertainties in sample-based estimates can be calculated for BBI inventories; however, a systematic analysis of uncertainties in the inventory estimates is not currently performed (for either planning or safety basis purposes) nor is such a systematic analysis planned from available information.

Recommendations

Short-term

WRPS personnel in charge of the BBI should continue the work in coordination with those involved in characterizing waste tank information to maintain the most updated information for planning and safety analysis. Computer-based applications (e.g., the BBIM) are used to maintain and verify the information in the BBI; however, additional opportunities for automation and their potential usefulness should be evaluated. Given the importance of preserving and accessing the information generated by BBI, a corporate approach to development, maintenance, and verification of the BBI should also be evaluated. Because of difficulties in speciating chemical and radionuclide inventories for planning and safety analysis purposes, the use of thermodynamic codes and databases (e.g., OLI ESP) should be evaluated for ion/charge balance calculations that could provide better inventory estimates. This approach could also provide a better cross-checking procedure than that currently used based on free hydroxide calculations.

A systematic approach to estimate uncertainties in inventory estimates in the BBI should be developed as the first step in an overall approach to evaluate overall system uncertainties for planning purposes including assuring that a sufficiently broad composition space is defined for glass testing and acceptance. These uncertainties should be characterized and documented in a systematic and transparent fashion based on available information and should be able to incorporate knowledge when new processing facilities (PT, WTP, etc.) are brought online.

Mid-term

If found necessary, thermodynamic codes and databases (e.g., OLI ESP) should be included in the calculations underlying the BBI estimates ion/charge balance calculations. The capability for generating consistent inventory uncertainties for both planning and Safety Analysis purposes should be provided. This capability could be provided either as part of the existing BBI report and underlying calculations or as a separate system and report; however, thought should be given to integrating these capabilities to the extent possible.

Long-term

The need for improved computational tools for estimating tank inventories and characterizing inventory uncertainties for potential use in optimizing the planning process should be investigated. The BBI, uncertainty estimates, and planning models should be integrated to the extent practical to allow propagation of inventory uncertainties for both planning and safety analysis purposes. The manner in which computations are performed for uncertainty and sensitivity analyses will impact the interactions among the various databases and tools. ORP should evaluate new computing environments for long-term planning needs including optimization under uncertainty.

6.2 Tank Waste Information Network System (TWINS)

Description

The Tank Waste Information Network System (TWINS) contains the official data characterizing Hanford tank wastes, including waste physical property data, sample data, and estimates of phase-based inventories and concentrations for approximately 80 species of interest [PNNL]. TWINS is programmed using Microsoft® SQLServer and .Net technologies and provides a common user interface (Figure 6.2.1) to 16 heterogeneous relational databases with 14 million records and a document repository of more than 4000 reports. TWINS provides a set of tools that can be used to review and select data (including the BBI described in the previous section) for planning purposes.

Figure 6.2.1 The Tank Waste Information Network System (TWINS) provides a common user interface to 16 supporting databases [PNNL].

TWINS provides entry, storage, report, editing, and network access capabilities for tank characterization data including inventory, analytical, sampling, vapor, and physical properties data for selected chemical and radionuclide species [ADAMS]. TWINS provides Internet access to data, documents and templates, graphics, standard data reports, and other information and includes the ability to perform key-word and tank-specific searches. System capabilities are frequently updated in response to user needs under the pertinent software QA program

[BANNING 2008a, BANNING 2008b]. TWINS is designated QA Level B software although some information (i.e., SOF and ULD factors) is QA Level A. Waste tank data is kept current to comply with Tri-Party Agreement (TPA) requirements [USDOE].

As illustrated in Figure 5.2.1, a common use for TWINS is to supply the Best Basis Inventory and wash and leach factors needed to run an HTWOS simulation [KIRKBRIDE 2009a, KIRKBRIDE 2009b]. HTWOS is a dynamic event-driven simulation that is used to predict and track the movement of tank waste throughout the River Protection Project (RPP) mission including storage, retrieval, processing and disposal steps to help form the technical basis for project schedules and programmatic planning.

Observations

TWINS successfully stores and provides, among other information, the official tank characterization data, wash and leach factors, and standard reports necessary to support design, tank farm operations, and planning purposes. This tool is currently being updated to take use of more modern programming tools and to remove QA Level A information (i.e., SOF and ULD factors) from TWINS; these factors are being moved to separate Level A spreadsheets. WRPS is also taking over the management of TWINS including updating security requirements and making outputs available outside the PNNL Local Area Network (LAN).

The Best-Basis Inventory (BBI) information and wash and leach factors provided by TWINS are often highly uncertain; the inventory uncertainties were considered in the previous section on the BBI. WRPS is currently evaluating methods to improve the wash and leach factors by using thermodynamic models and additional experimentation. Currently the uncertainties in inventories and wash and leach factors are either not considered or applied in a non-systematic fashion during planning.

Recommendations

Short-term

Because of the potential for Complex-wide application, a corporate approach to tank inventory management similar to other DOE inventory tools (e.g., LANMAS and NMMSS) should be considered. These changes will help reduce any potential impacts from future funding uncertainties on continuing development and maintenance. The information is TWINS is critical and must be preserved regardless of contractor changes.

A systematic approach to estimate uncertainties in the wash and leach factors (similar to that suggested in the previous section for the inventory estimates in the BBI) or solubility model predictions should be developed as part of an overall approach to evaluate system-level uncertainties for planning purposes including assuring that a sufficiently broad composition space is defined for glass testing and acceptance. These uncertainties should be characterized and documented in a systematic and transparent fashion based on available information and should be able to incorporate additional knowledge as it is obtained.

To help reduce the uncertainties in the wash and leach factors, an improved approach should be evaluated to estimate the degree of solubilization in the relevant leaching and washing processes. The details of the approach needed to significantly improve the wash and leach factors depends on the manner in which the tank farm and pretreatment processes will the operated (e.g., caustic concentration, temperature, solid/liquid ratio, etc.). The various thermodynamic codes and databases that are available should be evaluated for their potential to improve or replace these factors and to guide the additional experimentation needed to help validate their use.

Mid-term

Based on the requirements documents developed by the sites (in the short term), the integrated database system would be developed using the resources provided by DOE. The system can be tailored to the individual site's needs.

The logic necessary to incorporate improved wash and leach factors (or improved relationships) should be developed and incorporated into the integrated database. The capability to generate uncertainties associated with the wash and leach factors for planning purposes should be provided in the integrated database.

Long-term

Improved computational tools should be developed for characterizing the uncertainties important to the planning and safety analysis processes and for optimizing planning. A platform should be developed that provides the uncertainties needed for both planning and safety analysis. The analysis of uncertainties in these processes can, for example, take the form of error propagation studies. Provide a computing environment for long-term corporate knowledge continuation.

6.3 Hanford Tank Waste Operations Simulator (HTWOS)

Description

The Hanford Tank Waste Operations Simulator is a dynamic flowsheet and mass balance model used to simulate the RPP mission. The code is written in the Gensym G2 software and is run on Dell XPS 720 H2C workstations and Precision M90 laptops equipped with Windows XP SP3. The model has been run to test specific tank waste retrieval flowsheets and to assist in planning of near-term transfers, evaporator operations, baseline change requests, and project planning. It is used to validate the plans and to evaluate technical and programmatic assumptions for internal consistency. In addition to tank waste processing operations, the model also predicts the impact of changes to the system plan on the overall mission.

The major systems modeled by HTWOS include SSTs and retrieval facilities, DSTs, the Tank Farm evaporator, WTP Pretreatment operations, the LAW and HLW melters and off-gas systems, effluent treatment systems, supplemental waste systems, and waste disposal, as shown in Figure 6.3.1[KIRKBRIDE 2009c] The model is both continuous and event-driven. Specific operations, such as tank transfers, are modeled continuously until complete. Once the operation is completed, the subsequent event or activity is selected based on an evaluation of the exiting conditions of the pertinent facility. HTWOS is an objected-oriented programming code that uses knowledge base (KB) workspaces to organize data, operations, definitions, items and objects, which are represented graphically and manipulated through a Graphical User Interface (GUI) [KIRKBRIDE 2009c].

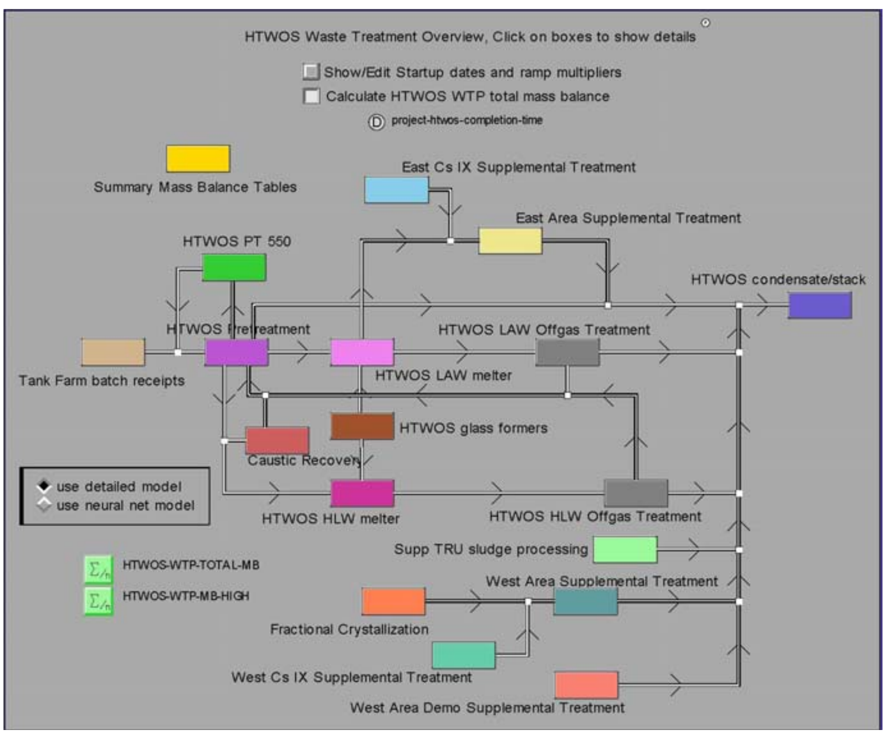


Figure 6.3.1 Waste Treatment Overview Workspace Illustrating the HTWOS GUI [KIRKBRIDE 2009c]

The inputs to HTWOS are the Best Basis Inventory, the near-term history of tank waste transfers, radioactive decay data, Wash and Leach Factors, process split factors, extents of reaction, and both HLW and LAW glass models. The HTWOS BBI report from TWINS is updated quarterly. Figure 6.3.2 lists the inputs and outputs for the model [KIRCH]. HTWOS saves model files, data, and results for each run in knowledge base (KB) files, model snapshots, and CSV data files. The HTWOS2XL application within G2 generates twelve verified Excel spreadsheet files for specific end users. These Excel files include transfer files, production plots, a summary mass balance, SST retrievals, WTP feed assessments (specifications 7, 8, HGR, and criticality), the quantity of HLW generated, the residual waste inventory, evaporator operations, and DST transfers. The HTWOS code also generates the feed vector for the WTP Dynamic Flowsheet model, which is also written in G2. The QA level for the software is Level F.

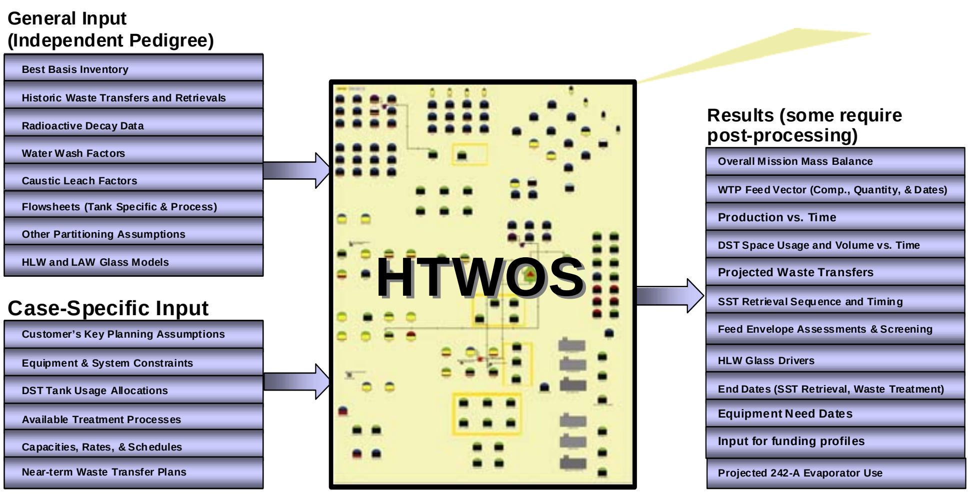


Figure 6.3.2 HTWOS Inputs and Outputs [KIRCH]

Observations

HTWOS has been used effectively for short-term and preliminary long-term planning for the River Protection Project Mission. The code models waste transfers and retrievals, evaporator operations, and WTP operations. It is also used to generate feed vectors for the WTP Dynamic Flowsheet (G2) model; however, the models are not directly interfaced. The WTP model within HTWOS is a simplified version of the stand-alone WTP Dynamic Flowsheet model, as it is used for planning of overall liquid waste management operations rather than management of the detailed operations within the WTP. Because of the time lag in implementation of changes to the WTP design, HTWOS uses older assumptions for WTP operations than does the WTP Dynamic Flowsheet model. The WTP design is evolving and resides with a different contractor, which limits HTWOS code ability to respond to changes in a timely fashion.

There are limitations associated with HTWOS as currently applied to the RPP mission. The model does not explicitly include any kinetics for the treatment reactions, nor does it include any thermodynamic data related to waste chemistry. Most chemistry is based on stoichiometric reactions with pre-defined extents of reaction. An additional limitation is the lack of detailed speciation information. The leach and wash functions are defined by water Wash Factors (WF) and caustic Leach Factors (LF). WRPS personnel are investigating new methods for handling solubilities in the model, including the use of the neural networking capability within the G2 software.

HTWOS model assumptions are based on the current WTP performance contract and upon ORP's assessment of how well the WTP may perform. Scenario development requires between days and months depending on complexity of modifications to the flowsheet. Actual run time is much less, requiring several hours to model a complete tank treatment campaign. In order to reduce calculation time, WRPS is exploring more powerful computing environments, and, to that end, recently purchased more powerful work stations to house the software. V & V is conducted by in-house modelers.

In terms of operational analysis, the model is not used to conduct cost-related analyses of operations. There is no explicit reliability analysis and equipment downtime and process upsets must be included explicitly in scenarios or accounted for by time-scales allotted for operations. The model does not currently handle uncertainties in tank compositions or in retrievals and transfers. The initial SST retrieval sequencing strategy is based on expert judgment. The biggest risk in feed delivery, rheology, is not currently addressed by modeling.

The HTWOS model is maintained by one chief modeler with two other trained HTWOS modelers. The modeling team includes several other engineers involved in system planning, but does not include any computer scientists. Access to HTWOS is controlled through the implemented HLAN policies, user-specific permissions to shared drives and areas, and the need for G2 software license keys.

Recommendations

Short-term

WRPS should investigate a better way to handle the solubilities of different waste components in the HTWOS model. This can be achieved by improving the calculation of the wash and leach factors or by implementing a better method to calculate solubilities directly. As rapid turnaround is critical to evaluation of tank retrieval and waste production scenarios, the RPP should continue to explore more powerful computing environment to speed calculations, whether through more powerful computers, as is currently being done, or through different computing environments. Apparently, running the HTWOS model on a Linux platform has the potential to speed calculations and, if desired, operate the model on more capable hardware. As the costs associated with changes to the scenarios are critical to the mission, the viability of incorporating cost estimates into the model should be evaluated. A formal effort should be made to begin to reconcile differences between WTP Dynamic Flowsheet (G2) model and HTWOS WTP assumptions. Because of the large uncertainties associated with tank compositions and their potential impact on downstream operations, WRPS should explore incorporation of uncertainties into calculations of compositions and transfers. Tracking of uncertainties throughout the process mission should provide planners with a much better method for evaluating competing options. Finally, an iterative approach based on glass acceptance and/or feed specifications should be developed in order to better identify alternative retrieval sequences and blending strategies.

Mid-term

In the middle term, an improved method to estimate the solubilities of waste components should be incorporated into HTWOS, whether derived from the wash and leach factor calculations or by more rigorous chemical or thermodynamic models. Uncertainty estimates should be incorporated into model for critical systems. Differences between the assumptions used for the WTP Dynamic Flowsheet model and the WTP model within HTWOS should be reconciled. If both models will be maintained, HTWOS should be a synchronized with the WTP Dynamic Flowsheet model.

Long-term

Consolidate G2-based models. Implement additional lifecycle evaluation functionalities (e.g. a cost module) if G-2 platform is appropriate.

6.4 WTP Dynamic Flowsheet Model (G2)

<u>Description</u>

The WTP Dynamic Flowsheet model "G2" is a dynamic flowsheet and mass balance model that is used to simulate WTP operations. The code is written in Gensym G2 (version 8.1) software running on MS Windows. The data generated by the model is stored and managed using ORACLE databases. The WTP Dynamic Flowsheet model performs discrete-time material balance calculations over the entire WTP based on the defined initial conditions, bounding conditions and logical sequencing of operations. The software Quality Assurance level is F, Non-Quality Affecting Software.

The performance of each unit operation is event-driven, adjusting periodically according to specified logic procedures corresponding to its condition or changes in process status. Figure 6.4.1 shows the model overview of WTP operations. All calculations simulate 6 min time intervals within the plant; one-minute time steps are used in the glass former reagent system to adequately capture process dynamics. Data can be transferred simultaneously to Oracle through bridges as the model runs.

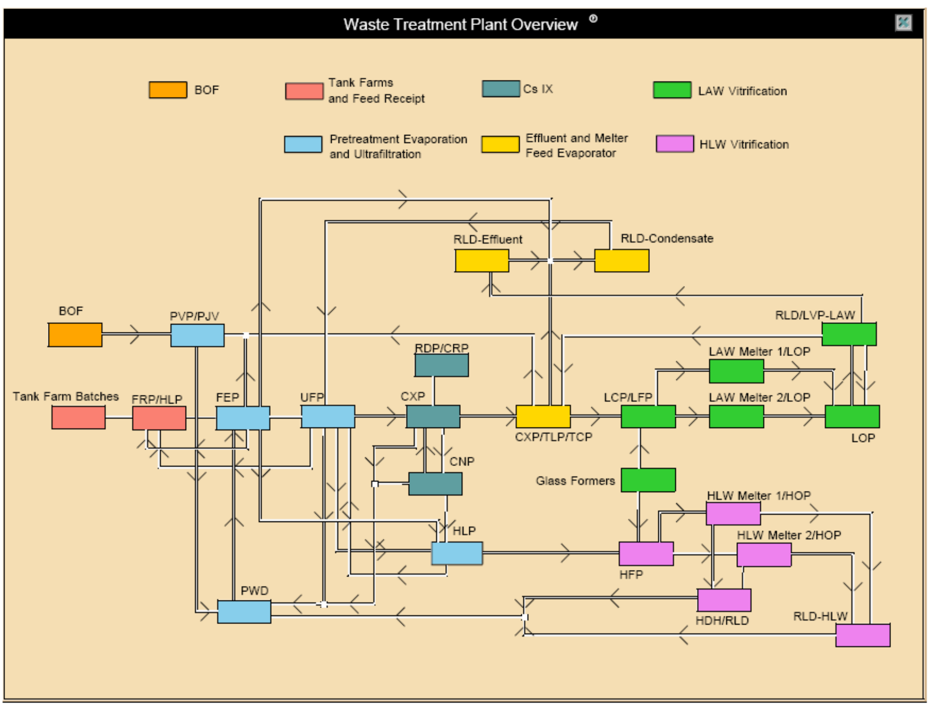
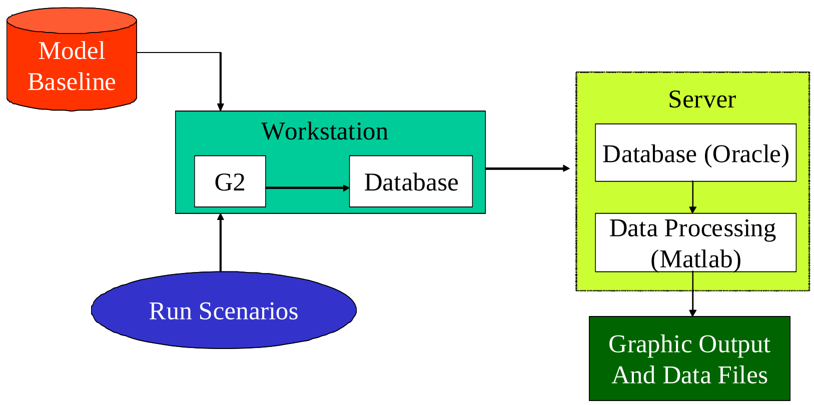


Figure 6.4.1 Workspace Showing Overview of WTP Operations [DENG]

The input to the Dynamic Flowsheet model is the HTWOS feed vector (ORP/TFCOUP), model baseline and run scenarios, and assumptions from the Model Design Document (MDD) and Bases, Assumptions, and Requirements Document (BARD) documents. The feed vector is imported directly from an Access database. It contains information on waste quantities and compositions, and on the leach factors for pretreatment operations; the composition is charge balanced and adjusted to meet requirements of WTP operations using G2MBC [DENG]. The outputs are given by process stream and include: volumes, solids, Na concentrations, totalizer data, glass property data, evaporator data, chemical additions, and mass balance data. Data can be written in intervals corresponding to multiples of 6 minutes. The output is processed using Oracle and Matlab and is in a form conducive to export to Excel spreadsheets. Figure 6.4.2 shows the data management configuration for the WTP Dynamic Flowsheet model [LEE 2009a].



6.4.2 Flowsheet Data Flow for the WTP Dynamic Simulation [LEE 2009a]

Observations

The WTP Dynamic Flowsheet model enables calculation of the detailed material balance of the complete WTP throughout mission. The constraints on IHLW canisters, throughput, Supplemental LAW, etc. as well as the feed vector for mission planning are driven by ORP. The results of the models yield assessments of tank utilization, the quantities of ILHW and ILAW generated, and the overall and specific plant capacity. The output serves as a framework for comparing operating options. The model output also serves as a point of comparison for other models, namely HTWOS. Automation of data input and output is effective, requiring minimal manual manipulation, and as such data management is not a time-consuming function. Similar to HTWOS, the WTP Dynamic Flowsheet model requires from several days to weeks to set up and run a model.

The glass output predicted by the WTP Dynamic Flowsheet model and HTWOS compare well for cases where the pretreatment process is limiting. The material balance is calculated but the model contains limited chemistry. Tank heels are accounted for in the model, and the calculated mass balance accounts for 99% of mass in the system, with the missing fraction ascribed to minor components. As with HTWOS, there is no description of downtime; availability is captured for the global system rather than for individual units, and process upsets must be included explicitly in scenarios or accounted for by the time allotted for operations. Downtime is captured in the Operations Research model rather than the WTP Dynamic Flowsheet model.

The WTP Dynamic Flowsheet model has several limitations related to chemistry and operations. The model allows exploration of different operating assumptions, including leach logics and kinetic expressions; however, all chemistry is based on stoichiometric reactions. There is no capability to model thermodynamics, and as a result, leach and wash functions are defined either by constant Wash and Leach Factors or by simple expressions. For example, the amount of caustic addition required for each batch in the WTP is currently estimated by an expression for free hydroxide concentration as a function of aluminum solubility which was obtained by a curve fit of experimental data in the literature. The model does not include prediction of chemical speciation. In terms of operation, there is no cost-related analysis. The process for selection of 6 and 1 minute time steps was not described.

Because G2 is not backward compatible, old versions of the model cannot be run on newer versions of the software. Validation and verification are done in accordance with the approved V&V Test Plan. Verification is typically performed by hand or using a spreadsheet by Process Flowsheet Modeling and Analysis personnel that are not associated with the WTP Dynamic Flowsheet model work, or by an individual involved in model development with Process Engineering and Technology (PET) management approval

Recommendations

Short-term

An improved method to model the solubilities of different waste components in the WTP Dynamic Flowsheet model should be developed by improving the calculation of the Wash and Leach Factors by calculating solubilities directly, or by linking to other predictive tools. The estimation of solubilities within the model should be explored. In order to accelerate evaluation of operating scenarios, a more powerful computing environment should be procured to increase productivity by improving availability and increasing the speed of calculations. Addition of modeling personnel would also improve turnaround time.

Differences in assumptions between the WTP Dynamic Flowsheet model and HTWOS WTP should be reconciled. Development of a systematic approach to convey changes in process flowsheets and operations to WRPS would reduce the chance for disparities. The incorporation of uncertainties in compositions and transfers should be pursued to enable the propagation of uncertainty through the plant and enable a better evaluation of competing processing options. If not already done, a systematic assessment of time step selection should be completed and documented.

Mid-term

In the middle term, an improved method for predicting solubilities should be implemented into the WTP Dynamic Flowsheet model calculations. The method selected should be reconciled with that developed for HTWOS and TWINS. Uncertainty estimates should be incorporated into model for critical systems. Differences between the assumptions used for the WTP Dynamic Flowsheet model and the WTP model within HTWOS should be reconciled.

Long-term

Consolidate G2-based models. Implement additional lifecycle evaluation functionalities (e.g. a cost module) if G-2 platform is appropriate.

6.5 Aspen Engineering Suite (AES) Steady-State WTP Model

Description

The Aspen Engineering Suite consists of a collection of process models written on a commercial platform developed by AspenTech. The software runs on 14 networked PC work stations. A fifteenth computer stores the run-time licenses for the AspenTech software. A diagram of the configuration is shown in Figure 6.5.1 [LEE 2009b]. The suite consists of four different codes: Aspen Custom Modeler (ACM), Aspen Plus®, Aspen-OLI, and Aspen Partition Controller. The latter software was developed specifically to manage the networked computers.

The Aspen Engineering Suite generates a steady state flowsheet model of the WTP. The flowsheet reconciles data using rigorous chemistry models of a number of operations within the WTP including the feed evaporator; the LAW evaporator; and the ultra-filtration, cesium ion exchange, off-gas treatment, and acid recovery systems. The model uses a tiered approach. The upper tier is written in ACM with four partitions, while the lower tier contains nine rigorous AspenPlus® models interfaced through Aspen Partition Controller. The partitions define two pretreatments: (1) caustic leaching and evaporation, and (2) cesium ion exchange, LAW processing, and HLW processing. The partitions are in place to improve run-time, selection of convergence criteria, and to simplify recycle calculations.

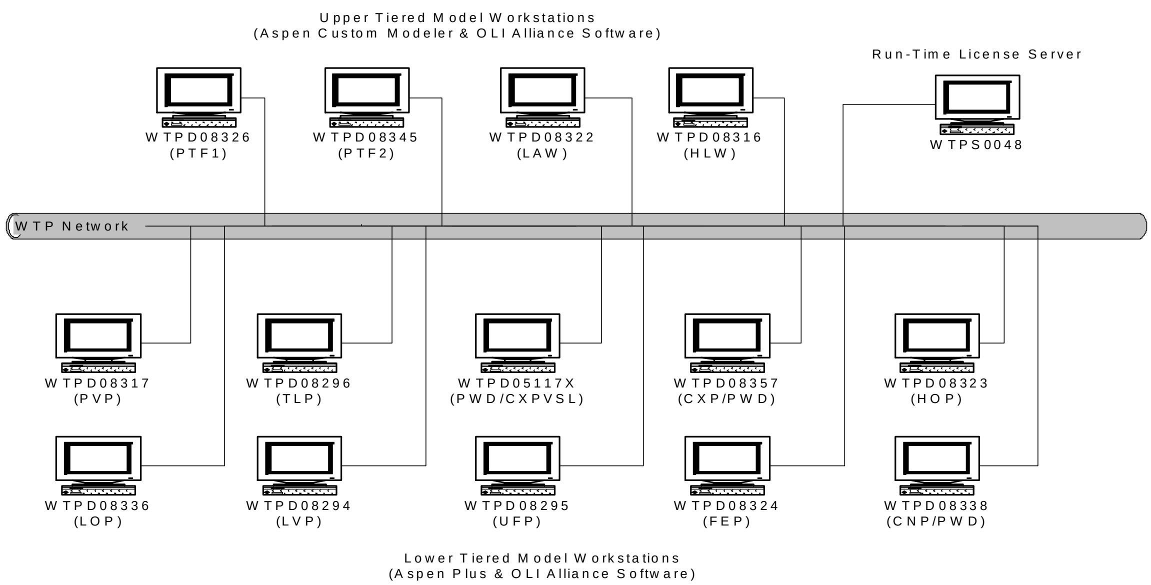


Figure 6.5.1 Workstation Configuration for the AES Model [LEE 2009b]

The lower tier models are aligned with the four ACM upper-tier partitions and provide more detailed calculation of processes within the upper tier flowsheets [DAVIS]. The first pretreatment partition is interfaced with lower tier AspenPlus® models for the feed evaporator and caustic leaching processes. The lower tier models for the second pretreatment partition include detailed models of the cesium ion exchange, nitric acid wash and evaporation processes.

The lower tier includes models of the treated LAW evaporator and off-gas processes, while the HLW model includes melter off-gas processing. The suite can be run in tiered or non-tiered mode. A number of simplified ("Reduced") process models and simplifications are used to run the model in the non-tiered model.

Inputs to the AES model are the data from the Hanford tank waste characterization and process verification testing. Physical properties data for the components are obtained from OLI's Environmental Simulation Program (ESP) and the WTPBASE chemistry databank. To date, three different tank chemistries have been reconciled. Outputs from the model include Excel spreadsheets listing composition and physical properties data for each process stream as well as fixed variables and constraints for each of the partitions. The software QA level is F, Non-Quality Affecting Software.

Observations

The AES Model provides detailed flowsheet chemistry for the WTP. None of the other planning models examined, such as the WTP Dynamic Flowsheet model or HTWOS, were capable of modeling the chemistry to the same degree. The AES Model was also the only model reviewed that is used to support the design effort. Because of the detailed chemistry, the model input includes detailed speciation for each of the feed compositions examined. Only three tank feeds have been reconciled with rigorous thermodynamics [JAIN]. Thus the flowsheets developed are specific to those tank wastes and must be redeveloped for any additional feed compositions. As a result, changes to the flowsheet are time and computationally intensive for planning purposes. There are limitations on converting element-specific inventory into speciated charge-balanced thermodynamic models, and AES may not be capable of handling all of the wastes that are to be received at the WTP due to limitations of the available thermochemistry databases. The model calculates processes at steady-state, so the output is a time-averaged mass balance calculation that approximates time varying processes, such as the cesium ion exchange.

There are several practical limitations on more extensive utilization of the AES model. There is currently only one full-time modeler who can run the code; one other modeler is available on a part-time basis. The organization also lacks the ESP expertise that is required to develop and run the program and must use outside sources such as PNNL and SRNL for expertise. Industry support is also somewhat limited; because of the unique nature of the application, developments are not suited to other customers. The model currently requires 15 linked work stations to run. Although this does not appear to limit the run-time of the model significantly, periodic network-related shutdowns and maintenance requirements do hamper running the model. Tests of the model on a single system with fourteen or more processors have shown that usage would improve if the system was decoupled from the network.

Recommendations

Short-term

In order to improve usage, the simulations should be run on a single machine with multiple processors (e.g., multi-processor blade workstation). Additional modeling resources are required particularly for AES and ESP due to the time required setting up and running the model. Ready access to subject matter experts would also improve preparation time, enabling additional compositions to be run, to increase confidence in the chemistry of the operations with the WTP.

To benefit from additional expertise, ORP should consider site-wide Aspen and OLI licenses that cover all contractors, and provide site wide access to WTPBASE and other relevant databases. DOE should also explore additional opportunities to advance thermodynamic modeling by engaging industry, academia, and national laboratories through an EM-wide effort to expand experimental studies and model development, and by continuing to support on-going studies, such as those at Mississippi State University.

Mid-term

In the middle-term, thermochemical properties databases should be expanded to ensure the capability to handle all tank wastes in AES and other models. Modern computing capabilities should be utilized to the extent feasible to boost run efficiency.

Long-term

In the longer term, DOE should consider a sustained effort to support the advancement of knowledge in chemical kinetics and thermodynamics. This area is critical to the development of models for nuclear applications and would benefit modeling efforts across a number of DOE missions and office. EM is in the particularly unique situation of maintaining access to field data throughout its mission that can be used to support the validation and testing of these models, and of benefiting from the higher fidelity designs and planning models that will result.

6.6 WTP Operations Research (OR) Model

Description

The current WTP contract requires Bechtel to develop and use process models to perform flow sheet RAM analyses and pre-operations assessments, and the WTP Operations Research (OR) Flowsheet model is the primary tool used for this purpose. The current model, version 5.0, was released in December 2008 and uses the WITNESS code. It includes the modeling of solids, liquids, vessels, and components in HLW and LAW, Pretreatment, and Analytical Laboratory (LAB) facilities, as well as the Glass Former Storage Facility. The WTP OR Model is generic enough to allow user modifications to customize “what-if” scenarios to provide quantifiable answers so management can provide specific recommendations. The model incorporates reliability, availability, and maintainability data to estimate plant availability over time. In addition, the model is used to monitor component failures and utilizations, estimate the facility throughput, and perform “what-if” scenarios based on the current engineering design. The WTP OR Model is routinely updated and improved to reflect the latest design and incorporate the latest information from the Research and Technology group. This update incorporates 14 model change requests (MCRs). Facilities are modeled with both discrete-event and continuous elements. Version 5.0 incorporates applicable information from the BARD, Operations Research Model Requirements [PEREDO], and from the Waste Treatment Plant RAM Basis Report [WADDELL].

Observations

WITNESS provides an “integrated plant availability”. As per contract, overall WTP availability should be 70% or 75%, depending on throughput. Separate OR models are being developed for WTP and the WFRD system by different organizations (i.e. WRPS plans to implement a WITNESS model for tank farm operations). As a result, bottlenecks can occur at the interface between these models unless coordination is required by ORP. A noted observation is that if the OR model was implemented as is stated in its functional requirements documents, the WITNESS model should be incorporating not only full-plant unit operations, and lifecycle material movements, but also lifecycle cost analysis. If this was actually done (and is technically possible) then the WITNESS model may have the capability to replace both of the G-2 based “material movement models”, and answer questions posed by the HLW-IPT regarding overall lifecycle cost impacts.

The WTP OR model represents the entire WTP Flow sheet (i.e., waste pretreatment, CIX, Melter, etc.). The OR models material flows through subsystems, including RAM of those subsystems. Balance of Facility issues (e.g. site water and electrical power access) are ignored because of assumed high availability. WITNESS uses discrete and continuous model elements. Continuous processes include the glass former facility and tank waste flow-through; discrete processes include the mechanical handling systems and canister production. The model assumes that all necessary spares are available when equipment breaks down.

Reliability information is obtained from site experience and commercial sources (e.g., pump failure rates, etc.). It is essential for OR models to include the best information possible regarding equipment failure rates, or the model will not produce accurate results. Hardware failures are typically characterized by a "bathtub shaped" curve. The chance of a hardware failure is high during the initial life of the equipment, the failure rate during the rated useful life of the equipment is fairly low, but once the end of the life is reached, failure rate of equipment increases again. In the WTP OR model, there is a "4,000 hour" warm up time before the model produces results. This "warm up" time attempts to ensure that model results are based on normal operating values, and are not unduly influence by early equipment failures.

The WTP OR model is incredibly complex and incorporates hundreds of individual pieces of equipment and subsystems built from those individual pieces. It tries to account for unit operations, equipment and personnel interactions, and logical conditions that exist between operating systems. The WTP OR team has done an admirable job of attempting to accommodate all the equipment and processes in the WTP plant, and the documentation provided to us was in many cases very good. However, some questions have been raised regarding the sufficiency (accuracy and provenance) of estimates used in the model. Specifically, the Mean Time Before Failure (MTBF) and Mean Time To Repair (MTTR) estimates for hundreds of items are provided in the Model Design Document [PEREDO].

An evaluation of the "reasonableness" of that data with the supplied information proved difficult. Therefore, another document [WADDELL] was requested from WTP that provides the rationale for the MTBF or MTTR numbers. This report shows that a comprehensive review of the RAM information for components in the WTP has been conducted and documented. That is a positive sign. However, there is some concern regarding the actual MTBF and MTTR data values presented in the supplied documentation. This concern is based on a review of the Glass Former model that was developed by an external vendor and incorporated into the WTP OR model (the Glass Former model seemed to have more conservative parameter estimates) and a review of the Salt Waste Processing Facility (SWPF) OR model, which models similar unit operations and uses similar equipment, but seems to have more conservative MTBF and MTTR estimates. Further investigation of this particular issue (adequacy of MTBF and MTTR data) is beyond the scope of this review, but it is part of our team's charter to point out a potential problem in the "reasonableness" of estimates. The MTBF and MTTR estimates are the key elements in constructing and overall availability model, and it is the team's view that further research should be conducted regarding the appropriate level of conservatism for the WTP MTBF and MTTR parameter estimates, and research should be conducted to ensure sufficient redundancy is built into actual plant construction (e.g. providing parallel systems and minimizing single-point or common-mode failures).

Recommendations

Short-term

In the near term, implementation of OR software for the Tank Farm (Waste Feed Delivery Model) should be coordinated with the WTP version to ensure that the two can be easily integrated in the future. This will reduce likelihood of bottlenecks occurring at interface between models. The WTP OR model should be reviewed to ensure equipment MTBF and MTTR is realistic—that is based on real life "nuclear maintenance" and other pertinent experience. Also, the ability of WITNESS to forecast optimum canister production using the built-in optimization routine should be evaluated.

Mid-term

In the middle-term, both the WTP and Tank Farm OR models should “modularize” the representations of the systems under evaluation so that the addition or removal of systems does not require major rework of the models. The OR models should also incorporate availability of spares information, i.e. lead times, rather than assume 100% availability. If feasible, the optimal rate of canister production should be forecast using the built-in optimization routine.

Long-term

In the longer-term, “life-cycle” scenarios evaluations should be conducted, if feasible, including analysis of splits between HLW and LAW, waste loading, retrieval sequencing, and blending and their impact on detailed cost analysis. Consolidate the Tank Farm and WTP OR models into a single waste processing OR model.

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Appendix A – Biographies of Review Participants

Team Members

Monica C. Regalbuto, Lead. Dr. Regalbuto is the head of the Process Chemistry and Engineering Department in Argonne's Chemical Sciences and Engineering Division. She is an affiliated researcher with the Massachusetts Institute of Technology, Cambridge, MA and currently holds an IPA position with DOE-EM. Dr. Regalbuto has made key contributions to nuclear fuel cycle technology, beginning with the TRUEX process for removing transuranic elements from aqueous acidic solutions such as those found at DOE waste sites throughout the United States. She led the development of AMUSE, a computer model used by researchers to optimize processes for separating dissolved spent nuclear fuel. Under Dr. Regalbuto's leadership, Argonne conducted a highly successful demonstration of CSSX, a process for separating cesium-137 from high-level radioactive waste at DOE's Savannah River site. She maintains technical leadership in the development of advanced separations processes as alternatives for recycling spent fuel. Dr. Regalbuto is a key contributor to the development and demonstration of the UREX+ processes and pre-conceptual engineering design. Dr. Regalbuto's research supporting the development of nuclear fuel cycle technologies combines her experience in separations, computer simulations and proliferation resistance areas. In 2007 Dr. Regalbuto received both the Hispanic Engineer National Achievement Award Corporation (HENAAC) Professional Achievement Award and the American Nuclear Society (ANS) Jane Oestmann Professional Women's Achievement Award. Dr. Regalbuto's publications include over 30 journal articles, reports and presentations and five patents. She received a B.S. from ITESM, Mexico and an M.S. and Ph.D. from the University of Notre Dame, IN.

Kevin G. Brown. Dr. Brown is Senior Research Scientist in the Department of Civil and Environmental Engineering at Vanderbilt University. His research has been supported by the multi-university Consortium for Risk Evaluation with Stakeholder Evaluation (CRESP). Dr. Brown's current research focuses on life-cycle risk evaluation, model integration, and waste management issues related to proposed advanced nuclear fuel cycles and cementitious barriers for nuclear applications. Between 1986 and 2002 at the Savannah River Laboratory, he was recognized as a DOE Complex-wide authority in process and product control for high-level waste vitrification. His activities supporting the Defense Waste Processing Facility (DWPF) included: 1) optimizing waste loading, 2) modeling critical properties, 3) managing uncertainties, and 4) supporting variability studies and waste form acceptance. He served a similar role across the DOE Complex supporting vitrification projects at Idaho, Hanford, and West Valley. Dr. Brown spent 2002-2003 at the International Institute for Applied Systems Analysis (IIASA) in Austria where he estimated potential transboundary radiation doses from hypothetical accidents at Russian Pacific Fleet sites. They were the first such studies known in the West. Dr. Brown led the CRESP evaluation of life-cycle risks for the DOE Idaho Site Subsurface Disposal Area (SDA) where wastes contaminated with radioactive and hazardous materials were buried in pits, trenches, and soil vaults before 1970. He supported the corresponding risk evaluation for the Idaho Site Calcined Bin Sets containing high-level wastes. The results were presented to the Idaho Site Citizens Advisory Board (CAB), who strongly endorsed the clarity of the approach and the results. He holds a BE in Chemical Engineering, an MS in Environmental and Water Resources Engineering, and a Ph.D. in Environmental Engineering from Vanderbilt University.

David W. DePaoli is currently Group Leader of the Separations and Materials Research Group, Nuclear Science and Technology Division at Oak Ridge National Laboratory. David has worked at ORNL for over 23 years and has been involved in a wide range of chemical- and energy-related research and development projects, including demonstration of environmental-cleanup and waste-treatment technologies, basic research on separations employing external fields, and development of separation processes to recover materials for medical isotope production. For the past 12 years, he has been group leader of the Separations and Materials Research Group in the Chemical Technology and Nuclear Science and Technology Divisions at ORNL, which conducts fundamental and applied R&D aimed at applying chemical engineering principles to develop energy-related technologies. He is currently involved in efforts to develop advanced materials for electrochemical double-layer capacitors, devise new routes for production of chemical feedstocks from renewable sources, improve centrifugal contactor performance models for solvent extraction, and demonstrate real-time characterization tools for nanomaterials production processes. David has also been active in recent roadmapping activities for Nuclear Energy Advanced Modeling and Simulation (NEAMS) in the Department of Energy's Office of Nuclear Energy. David is Associate Editor for the journal *Separation Science and Technology*, and has acted as General Chairman for the 11th through 15th Symposia on Separation Science and Technology for Energy Applications. David has been an Adjunct Associate Professor in the Department of Chemical and Biomolecular Engineering at the University of Tennessee since 1999, and a director of the Separations Division of the American Institute of Chemical Engineers from 2003 through 2007. David received a BS in chemical engineering from the University of Michigan, and a Ph.D in chemical engineering from the University of Tennessee. He is author of over 40 peer-reviewed publications, and holds four patents.

Candido Pereira has been a researcher in the Chemical Sciences and Engineering Division of Argonne National Laboratory for the past 16 years. He received his PhD in Chemical Engineering from the University of Pennsylvania. At Argonne, he has worked on several programs related to the processing of spent nuclear fuel. In the Integral Fast Reactor program, he led efforts to develop an ion exchange process for cleaning spent salt from the electrorefining of spent metallic fuels to allow its recycle, and to develop a ceramic waste form for the sequestration of active metal fission product chlorides. He conducted research on the processing of gasoline and diesel fuel using catalytic systems to generate hydrogen for fuel cell applications. He currently conducts research on the treatment of spent commercial reactor fuel through the Advanced Fuel Cycle Initiative. He played a lead role in the UREX+ demonstrations that were run at Argonne between 2003 and 2007, authoring several summary reports. He has also worked on enhancing the AMUSE solvent extraction code, and on the conceptual design and simulation of an advanced spent fuel treatment plant based on the UREX+1a process. Recent research has also centered on the implementation of safeguards in spent fuel treatment facilities, both through AFCI and NNSA programs. He currently leads the Process Simulation and Equipment Design Group.

John R. Shultz. Dr. Shultz currently works in the DOE Office of Environmental Management but formerly worked in the DOE Office of Security, where he helped draft the DOE Safety Software Guide (DOE G 414.1-4) and provided input on the DOE Quality Assurance Order (DOE O 414.1C). For this work he received a commendation from the Assistant Secretary for the Office of Environment, Safety and Health (John Shaw). In addition, Dr. Shultz is acknowledge as a contributor to ANSI/ANS-10.4-2008 “Verification and Validation of Non-Safety Related Scientific and Engineering Computer Programs For the Nuclear Industry” and is currently on the standards development team for ANSI/ANS-10.7-200x; "Non-Real Time, High Integrity Software for the Nuclear Industry". While in the Office of Security, Dr. Shultz revised DOE M 474.1-2A, which governs the reporting of nuclear material inventories and transactions to the Nuclear Materials Management Safeguards System (NMMSS), a transaction-based, summary-level database of all nuclear material in the United States. Furthermore, Dr. Shultz was a member of an item-level nuclear material accountability software development team (Local Area Network Material Accounting System-LANMAS) that received the DOE CIO Technical Excellence Award. In addition, Dr. Shultz has worked with a team of DOE engineers and scientists to help the Russians design and implement a nuclear materials database and accountability system. Dr. Shultz was previously employed as a lead research engineer and senior policy analyst with the National Energy Technology Laboratory, US Department of Energy, Morgantown, WV where he published many technical articles, ran a research facility, and gained experience in power production, natural gas distribution, greenhouse gas production and mitigation, risk modeling, automobile emissions testing, particulate removal technologies, natural gas and oil extraction, and offshore production facilities. Dr. Shultz is a Certified Software Quality Engineer (CSQE) and a former active duty and reserve Army military policeman (enlisted) and engineer (officer).

Team Observers

<u>Sonitza M. Blanco.</u> Mrs. Blanco is the Team Lead for Planning and Coordination in the Waste Disposition Project at the U.S. Department of Energy Savannah River Operations Office. She is an industrial engineer with over twenty-two years of experience in project management, strategic planning and integration of radioactive liquid waste treatment and disposal facilities. She provided guidance and support in the development of the last two radioactive liquid waste disposition system plans and the development of discrete-event simulation models to simulate the different operating processes and systems in Liquid Waste Operations.

<u>Bob Chang.</u> Mr. Chang is a fellow engineer in the System Integration / Risk Management group at Savannah River Remediation LLC. He is a chemical engineer with over 20 years of experience in simulation modeling and analysis of complex nuclear chemical processes; in radioactive waste management; and in process engineering & development. His most recent assignment is in the area of system integration and planning of liquid waste operations; and he is working on developing a Liquid Waste Integrated Model. He was a lead of a modeling group in Systems Engineering and Integration department, responsible for developing models to identify improvement opportunities for various nuclear material/waste processing projects within Savannah River Site. Examples of cost benefits from the modeling effort are: (1) $1.2million dollars cost avoidance in the HB-Line Filtrate Tank Replacement project, and (2) $3-5 million dollars per year of cost avoidance by providing justification to stop ARP processing post SWPF startup.

Appendix B - Evaluation of System Level Modeling and Simulation Tools in Support of Hanford Site Liquid Waste Planning Process

1.0 Background

The Hanford Site, a 586-square-mile DOE Complex located along the Columbia River in the State of Washington produced nuclear material for national defense programs. Liquid wastes produced during the Manhattan Project and throughout the Cold War have been stored at the site's Tanks Farms. Approximately 57 million gallons of radioactive and chemically hazardous wastes are stored in 177 underground tanks located on Hanford's Central Plateau. The inventory was generated as a by-product of the recovery of plutonium from Hanford's nine nuclear reactors. Irradiated fuel from those reactors was transported to six separations facilities, where the use of multiple separation processes resulted in a wide variety of waste compositions. In the 1950s and 1960s, approximately one million gallons of liquid radioactive waste may have been inadvertently released into the environment.

From 1944 to 1989, the liquid waste was pumped as slurry from the separations facilities through underground transfer lines and stored in underground storage tanks constructed of carbon steel. Since the separations processes operated under acidic conditions, sodium hydroxide was added to the waste streams prior to transfer to inhibit corrosion. The entrained solids settled to the bottom of the tanks, creating a bottom layer designated as sludge and a clarified liquid above, the supernate. To reduce the total volume of waste stored, the supernate was periodically decanted, transferred out of waste tank farms, and evaporated. The concentrated slurry was returned to the storage tanks, where cooling resulted in formation of saltcake, a crystalline solid phase. Long-term storage at high temperatures has also resulted in the formation of a solid mass or groups of large solids that are not easily removed and so are referred to as "hard-to-remove" heels at the bottom of some tanks.

There are seven tank farms (86 tanks) located in the 200 West area and eleven tank farms (91 tanks) located in the East area. The tanks are of two main types: single-shell (SST) and double-shell (DST). Since 1980, the SSTs have not been in active service and all liquids have been transferred to the DSTs. As of July 2008, inventory estimates are: SSTs -- 30 Mgal and 95 MCi of radioactivity, mainly as dried sludge solids of saltcake containing entrained gases and interstitial liquids, and DSTs -- 27 Mgal and 95 MCi of radioactivity, mainly as liquids and settled solids (salts or sludge). An overall summary of waste tanks is given in Table 1. The DST space is carefully tracked because a portion of the DST space is reserved for contingency in the event a tank leaks and to accommodate safety operational constraints. The DSTs are an integral part of the River Protection Project (RPP) System Plan. Their mission is to:

- Support SST waste retrieval
- Support 242-A Evaporator operations
- Stage feed for delivery to the Waste Treatment Immobilization Plan (WTP)

Table 1. Hanford Waste Tanks Types

Type	Total Number of Tanks	Current Waste Inventory
SST	**149**	**30 Mgal**
Comments - Built from 1943 to 1964 and consists of large-capacity 133 (100 series) and 16 smaller-capacity (200 series) tanks. Assumed leaked 67. 83 are located in the West and 66 in the East 200 area. As of November 1980 all removed from active service. As of 2004 all interim (liquid removed) stabilized. As of April 2009, 7 have been retrieved, 3 have been retrieved to the limits of current technology and one is in the process.		
DST	**28**	**27 Mgal**
Comments - Built from 1968 to 1986 with an improved design and have never leaked. All tanks are currently active and subject to an integrity program. Three are located in the West and 25 in the East 200 area.		

The current plan for liquid waste processing consists of a number of highly integrated activities that require coordination among multiple contractors. Office of River Protection (ORP) manages two main contracts within the RPP system:

- The Tank Operations (TOC) Contract [DE-AC27-08RV14800] held by Washington River Protection Solutions (WRPS) includes the construction, operation, and maintenance activities necessary to store, retrieve, and transfer tank wastes; provide supplemental pretreatment for tank waste; and provide treatment, storage, and/or disposal of glass product and secondary waste streams.

- The WTP Contract [DE-AC-27-01RV14136] held by Bechtel National, Inc. (BNI) includes the design, construction, and commissioning of a pretreatment facility, two vitrification facilities (one for HLW and one for LAW), a dedicated laboratory, and supporting facilities to convert radioactive tank wastes into glass for long-term storage or final disposal.

In addition ORP interfaces with two DOE – Richland Operation Office (RL) contractors, the Mission Support Contractor and the Plateau Remediation Contractor, for waste disposal services, as well as some construction and ventilation work. Since RL is responsible for the groundwater under the tanks, it conducts the monitoring and planning. It is important to emphasize that each contractor manages facilities that are at different stages of development: (1) existing, (2) under design or construction, and (3) planned future. Alignment of program costs, scope and schedules from contractor's plans to individual facility operations is challenging. The current system plan [ORP-11242 Rev. 4 DRAFT] addresses these issues. Tank waste removal and treatment is a multi-year process that consists of the following steps:

1. Retrieving waste from the SSTs (*status: interim stabilized/retrieval in progress*), transferring to DSTs, (*status: operational*) and delivering the waste to WTP

2. Constructing and operating WTP. The WTP (*status: design and construction*) consists of three individual waste treatment facilities: (1) Pretreatment (PT), (2) High-Level Waste (HLW) Vitrification and (3) Low-Activity Waste (LAW) Vitrification.

3. Developing and deploying supplemental treatment capability is assumed to require a second LAW facility (*status: future facility*) that can safely treat about two-thirds of the LAW contained in the tank farms.

4. Developing and deploying treatment and packaging capability for Contact-Handled Transuranic (CH-TRU) tank waste (*status: early design*) for possible shipment to and disposal at the Waste Isolation Pilot Plant (WIPP) in New Mexico farms (*status: operational*).

5. Deploying interim storage capacity (*status: operational*) for the immobilized high-level waste (IHLW) pending determination of the final disposal pathway.

6. Closing the SST and DST tank farms, ancillary facilities, and all associated waste management and treatment facilities (*status: planning*).

7. Optimizing the overall mission (*status: planning*) by resolution of technical and programmatic uncertainties, configuring the tank farms to provide a steady, well-balanced feed to the WTP, performing trade-offs of the required amount and type of supplemental treatment and of the amount of HLW glass versus LAW glass.

The WTP contract covers the WTP construction and TOC contract covers the remainder, including WTP operation. The ORP mission has the challenge of retrieving and treating Hanford's tank waste and closing the tank farms to protect the Columbia River. Integration of facilities that are at multiple stages of development and manage by different contractors makes this challenge even harder. The RPP seeks to accomplish this by developing an integrated system plan shown in Figure 1.

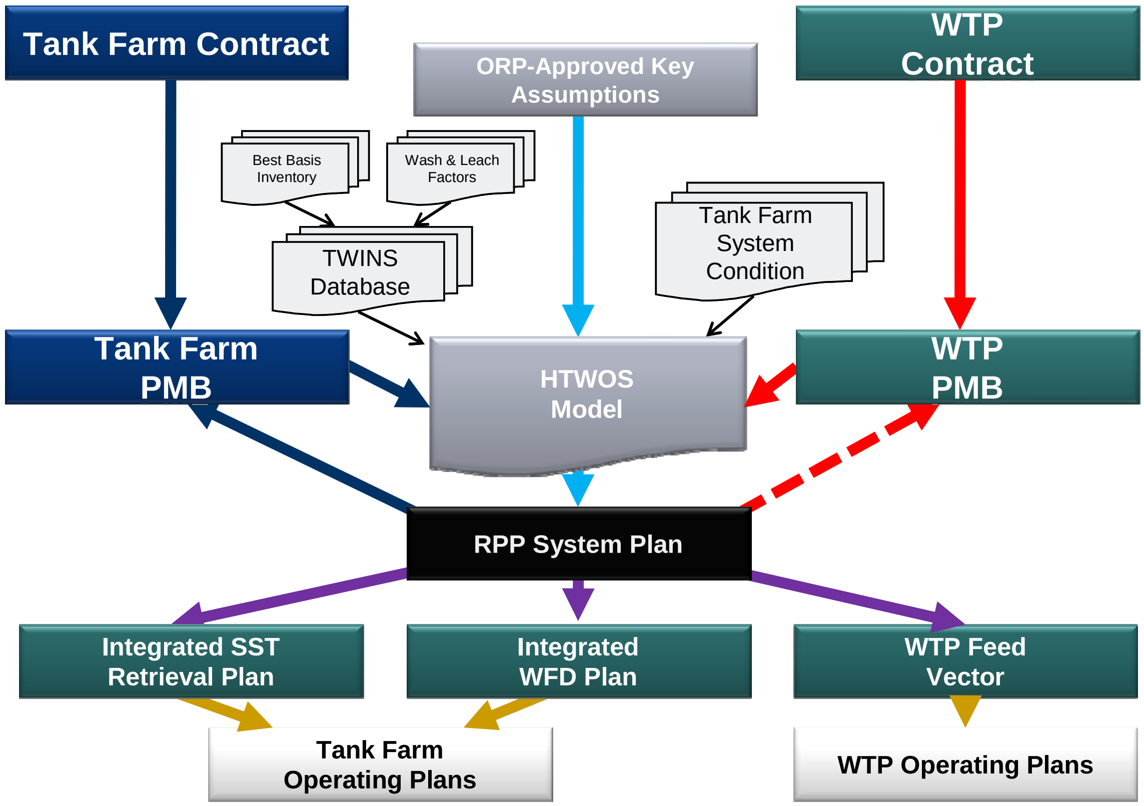

Figure 1. River Protection Project System Planning [ORP-11242 Rev. 4 DRAFT]

2.0 Scope of the Review

The objective of this review is to evaluate the current Process Simulation Tools that support the planning basis for the ORP Life-cycle Liquid Waste Disposition System Plan.

This review will focus on three primary areas:

- Assess the assumption that the tools used for liquid waste process simulation yield reasonable estimates. Evaluate methods used to model facilities that are currently in either design, construction or planning stages.
- Evaluate if additional tools are needed to guide actual execution of individual processing steps.
- Evaluate ability to timely update models as facilities in design, construction or planning stages refine their designs and operational envelopes.

3.0 Team Membership

The team will include five or more independent experts whose credentials and experience align with the specific lines of inquiry (LOI) listed below and who collectively provide to the team sufficiently broad capability and flexibility to address the full range of issues that may emerge in this review. Technical expertise includes, but is not limited to design, engineering and management of chemical processing and computer software development. Individual expertise and experience will be commensurate with the LOI. The experts must be free of any conflicts of interests with ORP.

Each team member is responsible for conducting a thorough, professional and independent review, for supporting the identification and resolution of technical issues, for participating in the development of draft and final reports, and for supporting resolution of comments and any points of disagreement. Collectively, the team is responsible for producing a high quality review report that is responsive to this charter, that includes unambiguous conclusions regarding the identified lines of inquiry, and that presents clearly any dissenting viewpoints. All team members will sign the final report.

Team members for this review:

Monica C. Regalbuto (EM-21)

Kevin G. Brown (Vanderbilt University and CRESP)

David W. DePaoli (ORNL)

Candido Pereira (ANL)

John R. Shultz (EM-21)

SRS Observers:

Sonitza Blanco (SRS)

Robert Chang (WSRC)

4.0 Period of Performance

This review will formally begin in early June 2009. The review shall include a combination of presentations, interviews with key personnel, information gathering sessions, independent document reviews, and group discussions. The review is expected to be completed at the end of July 2009. The key milestones for the review team are as follows:

- Provide Supporting Documentation — June 15, 2009
- Site Visit to SRS — June 29- July 2, 2009
- Status Briefing to EM Senior Management — July 6-10, 2009
- Team Meeting – Draft Report — July 24, 2009
- Final Report Approved by Team Members — July 31, 2009

5.0 Lines of Inquiry

Is there an adequate overarching strategy (master plan/schedule) developed to integrate all systems and operations under consideration that will be necessary for processing liquid waste ORP? A systems approach ensures that all operations and interfaces, risks and alternatives are evaluated to ensure that throughput, schedule and budget and other overall requirements are met. "Adequate" considers maturity of each aspect with respect to schedule; is the degree of development and planning sufficient to meet the schedule for implementation? What aspects of a systems approach are in place, and which aspects are missing?

- 5.1 How did ORP select the various software "tools" they are using?
- 5.2 Given the multiple contractors and stages of development of the facilities, how does ORP account for process unknowns?
  - 5.2.1 How are unknowns tracked and models updated as new information becomes available?
  - 5.2.2 How are new versions of the performance measurement baseline (PMB) for the tank farm and WTP integrated?
- 5.3 The Hanford Tank Waste Operations Simulator (HTWOS) has been identified as the center of the RPP system planning process. The model currently has some limitations. What are the effects on the System Plan Results of assumptions done by HTWOS regarding:
  - 5.3.1 Waste transfer systems, not accounting for operational limitations such as transfer equipment, settling times and tank space allocations
  - 5.3.2 Sodium management: adding as needed for corrosion mitigation and keeping aluminum in solution, but have the effects on the overall system been evaluated?
  - 5.3.3 Continually changing tank farms conditions
  - 5.3.4 Determination of glass acceptability
  - 5.3.5 Continually changing glass formulation for HLW and LAW
  - 5.3.6 Need for supplemental pretreatment capacity at WTP
  - 5.3.7 Limitations of water chemistry models which were developed for dilute systems and may not apply to current mission conditions
  - 5.3.8 Expanded operational feed envelope (outside of current range)
  - 5.3.9 Simplified representation of the WTP process
- 5.4 The HTWOS model requires input information from a variety of sources. What are the effects on the System Plan Results on assumptions made by the planning tools that provide the inputs to the model?
- 5.5 Does the Best-Basis Inventory (BBI) which provides waste characterization data adequately estimate the composition and inventory of the liquid waste tanks?
  - 5.5.1 What calculations are performed?

5.5.2 What are the pertinent data needed to perform the estimation?

5.5.3 How is gas generation calculated

5.6 Do the water-wash and caustic-leach factors adequately estimate the composition and inventory of the washes resulting from each sludge batch?

5.6.1 What calculations are performed in the spreadsheets?

5.6.2 What are the pertinent data needed to perform the estimation?

5.7 How does the Tank Waste Information Network System (TWINS) evaluate the information from BBI, water wash and caustic leach factors and the supplemental characterization data for use by HTWOS?

5.8 What is the confidence level of the feed vectors generated by HTWOS for input to WTP Dynamic Model (G2) and how is this confidence tracked?

5.9 The WTP G2 model is used for analysis and assessment of WTP operations: equipment utilization, reagent demand, process and facility design options, integration with tank farms and waste acceptance. If designs are frozen for regulatory license acquisition, how are these results used?

5.10 What is the relationship between HTWOS and G2?

5.11 Has the quality of the process simulation tools been adequately assured (i.e., is the QA plan adequate)?

5.11.1 What is the traceability of data used to support the models?

5.11.2 Has Validation and Verification (V&V) been conducted?

5.11.3 Are there any benchmark validation study reports?

5.11.4 How are version and revision controlled?

5.11.5 How are users instructed on software execution?

5.12 Are all critical processing steps characterized?

5.13 How do predictions produced by previous simulation tools compare with actual process performance?

5.14 How do the current simulation tool predictions compare with those from other tools used at other sites?

5.14.1 Have side-by-side comparisons been done?

5.15 Is the time required to conduct a study of model predictions acceptable for evaluation of project risks?

5.16 Is the current equipment available, number of licenses purchased, number of trained personnel adequate to perform the scope of modeling needed?

5.17 Is the output of models provided in a user friendly format (Graphical User Interface)?

6.0 Approvals

Mark Gilbertson, Deputy Assistant Secretary
Office of Engineering and Technology
Office of Environmental Management
FOR U.S. Department of Energy

6/18/09
Date

for Stacy L. Charboneau
Assistant Manager for Tank Farms Project
Office of River Protection
Office of Environmental Management
U.S. Department of Energy

6/17/09
Date